



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 09:03 am GMT

PDB ID : 4V7L  
Title : The structures of viomycin bound to the 70S ribosome.  
Authors : Stanley, R.E.; Blaha, G.  
Deposited on : 2009-11-12  
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

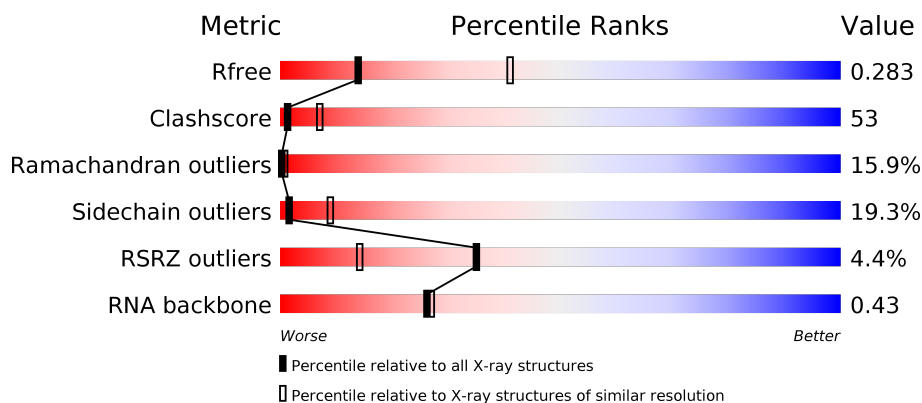
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1692 (3.00-3.00)                                      |
| Clashscore            | 112137                      | 2037 (3.00-3.00)                                      |
| Ramachandran outliers | 110173                      | 1973 (3.00-3.00)                                      |
| Sidechain outliers    | 110143                      | 1976 (3.00-3.00)                                      |
| RSRZ outliers         | 101464                      | 1716 (3.00-3.00)                                      |
| RNA backbone          | 2435                        | 1007 (3.34-2.66)                                      |

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. 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    | 1509   |                  |
| 1   | CA    | 1509   |                  |
| 2   | AB    | 256    |                  |
| 2   | CB    | 256    |                  |

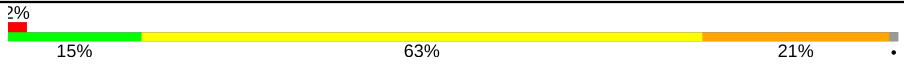
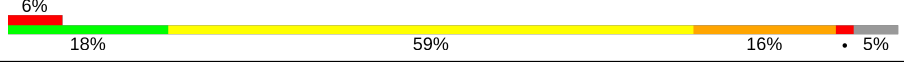
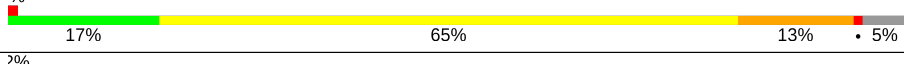
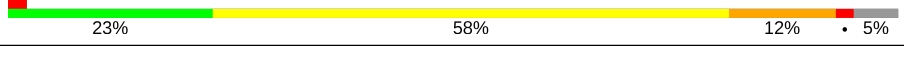
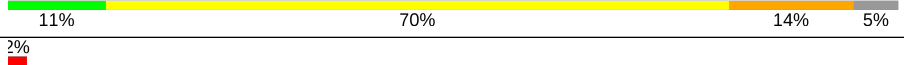
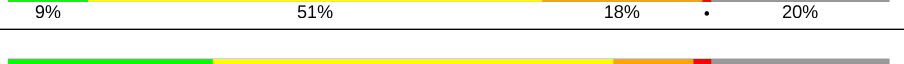
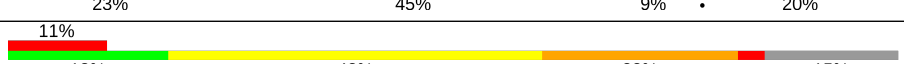
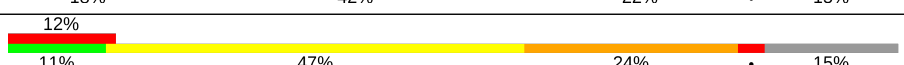
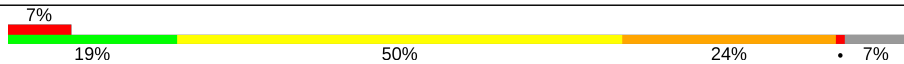
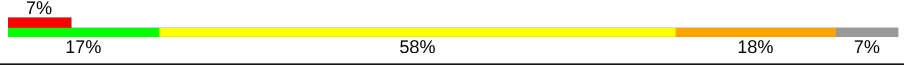
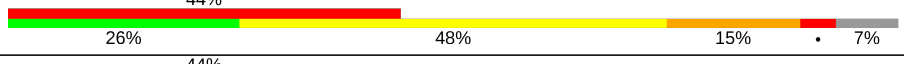
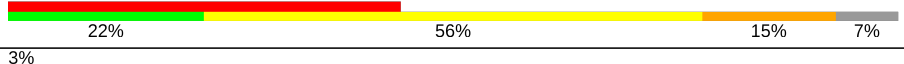


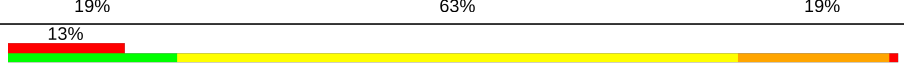
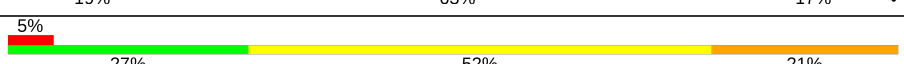
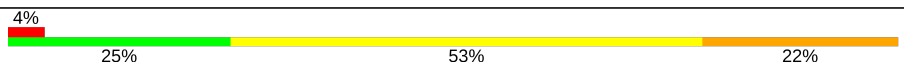

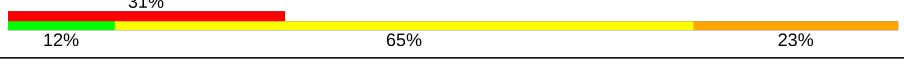






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | AC    | 239    |                  |
| 3   | CC    | 239    |                  |
| 4   | AD    | 209    |                  |
| 4   | CD    | 209    |                  |
| 5   | AE    | 162    |                  |
| 5   | CE    | 162    |                  |
| 6   | AF    | 101    |                  |
| 6   | CF    | 101    |                  |
| 7   | AG    | 156    |                  |
| 7   | CG    | 156    |                  |
| 8   | AH    | 138    |                  |
| 8   | CH    | 138    |                  |
| 9   | AI    | 128    |                  |
| 9   | CI    | 128    |                  |
| 10  | AJ    | 105    |                  |
| 10  | CJ    | 105    |                  |
| 11  | AK    | 129    |                  |
| 11  | CK    | 129    |                  |
| 12  | AL    | 132    |                  |
| 12  | CL    | 132    |                  |
| 13  | AM    | 126    |                  |
| 13  | CM    | 126    |                  |
| 14  | AN    | 61     |                  |
| 14  | CN    | 61     |                  |
| 15  | AO    | 89     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | CO    | 89     |    |
| 16  | AP    | 88     |    |
| 16  | CP    | 88     |    |
| 17  | AQ    | 105    |    |
| 17  | CQ    | 105    |    |
| 18  | AR    | 88     |    |
| 18  | CR    | 88     |    |
| 19  | AS    | 93     |    |
| 19  | CS    | 93     |    |
| 20  | AT    | 106    |    |
| 20  | CT    | 106    |   |
| 21  | AU    | 27     |  |
| 21  | CU    | 27     |  |
| 22  | AV    | 30     |  |
| 22  | CV    | 30     |  |
| 23  | AW    | 75     |  |
| 23  | CW    | 75     |  |
| 24  | AX    | 77     |  |
| 24  | CX    | 77     |  |
| 25  | AY    | 75     |  |
| 25  | CY    | 75     |  |
| 26  | AZ    | 6      |  |
| 26  | CZ    | 6      |  |
| 27  | BA    | 2915   |  |
| 27  | DA    | 2915   |  |


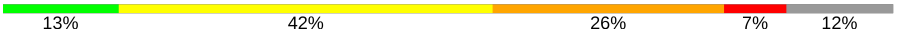


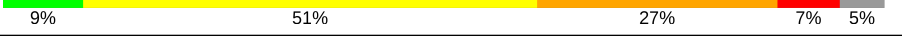
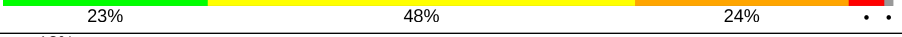
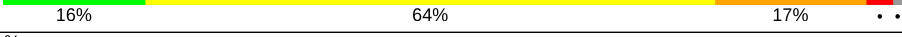

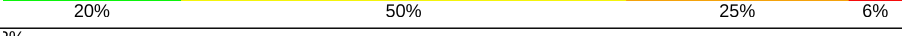

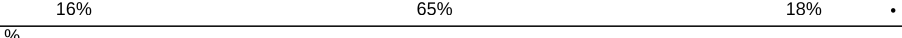
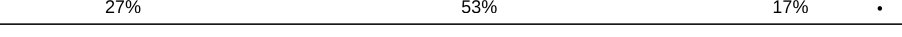
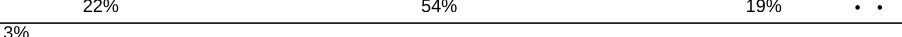
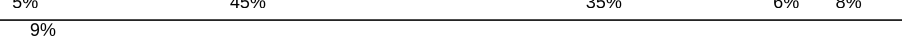


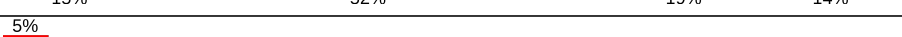
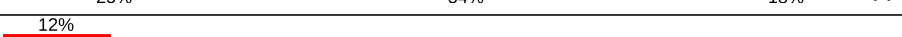
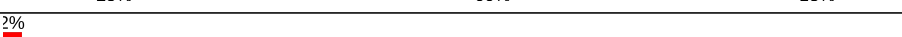
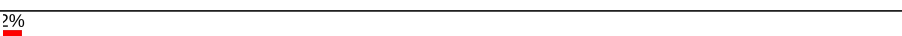

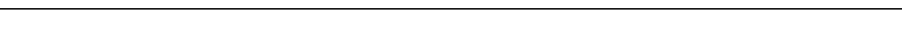
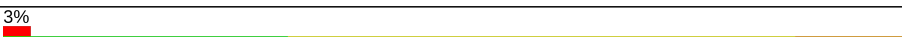
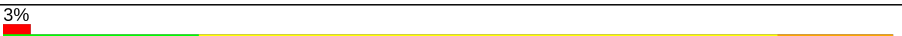

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | BB    | 122    |                  |
| 28  | DB    | 122    |                  |
| 29  | BC    | 229    |                  |
| 29  | DC    | 229    |                  |
| 30  | BD    | 276    |                  |
| 30  | DD    | 276    |                  |
| 31  | BE    | 206    |                  |
| 31  | DE    | 206    |                  |
| 32  | BF    | 210    |                  |
| 32  | DF    | 210    |                  |
| 33  | BG    | 182    |                  |
| 33  | DG    | 182    |                  |
| 34  | BH    | 180    |                  |
| 34  | DH    | 180    |                  |
| 35  | BI    | 148    |                  |
| 35  | DI    | 148    |                  |
| 36  | BN    | 140    |                  |
| 36  | DN    | 140    |                  |
| 37  | BO    | 122    |                  |
| 37  | DO    | 122    |                  |
| 38  | BP    | 150    |                  |
| 38  | DP    | 150    |                  |
| 39  | BQ    | 141    |                  |
| 39  | DQ    | 141    |                  |
| 40  | BR    | 118    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 40  | DR    | 118    |    |
| 41  | BS    | 112    |    |
| 41  | DS    | 112    |    |
| 42  | BT    | 146    |    |
| 42  | DT    | 146    |    |
| 43  | BU    | 118    |    |
| 43  | DU    | 118    |    |
| 44  | BV    | 101    |    |
| 44  | DV    | 101    |    |
| 45  | BW    | 113    |    |
| 45  | DW    | 113    |    |
| 46  | BX    | 96     |   |
| 46  | DX    | 96     |  |
| 47  | BY    | 110    |  |
| 47  | DY    | 110    |  |
| 48  | BZ    | 206    |  |
| 48  | DZ    | 206    |  |
| 49  | B0    | 85     |  |
| 49  | D0    | 85     |  |
| 50  | B1    | 98     |  |
| 50  | D1    | 98     |  |
| 51  | B2    | 72     |  |
| 51  | D2    | 72     |  |
| 52  | B3    | 60     |  |
| 52  | D3    | 60     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | B4    | 71     |                  |
| 53  | D4    | 71     |                  |
| 54  | B5    | 60     |                  |
| 54  | D5    | 60     |                  |
| 55  | B6    | 54     |                  |
| 55  | D6    | 54     |                  |
| 56  | B7    | 49     |                  |
| 56  | D7    | 49     |                  |
| 57  | B8    | 65     |                  |
| 57  | D8    | 65     |                  |
| 58  | B9    | 37     |                  |
| 58  | D9    | 37     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 26  | UAL  | CZ    | 5    | -         | -        | X       | -                |
| 26  | 5OH  | CZ    | 6    | -         | -        | X       | -                |
| 59  | MG   | AA    | 1603 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1619 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1622 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1637 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1640 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1665 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1677 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1697 | -         | -        | -       | X                |
| 59  | MG   | AX    | 105  | -         | -        | -       | X                |
| 59  | MG   | BA    | 3010 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3012 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3014 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3018 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3020 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3021 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 59  | MG   | BA    | 3023 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3024 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3047 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3050 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3056 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3066 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3081 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3088 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3091 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3095 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3106 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3115 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3120 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3128 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3134 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3151 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3154 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3161 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3183 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3188 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3189 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3192 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3193 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3194 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3199 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3213 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3216 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3223 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3251 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3295 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3336 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3337 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3341 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3345 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3381 | -         | -        | -       | X                |
| 59  | MG   | BU    | 201  | -         | -        | -       | X                |
| 59  | MG   | CA    | 1606 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1610 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1615 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1616 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1620 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1629 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 59  | MG   | CA    | 1633 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1639 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1642 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1663 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3002 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3003 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3005 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3007 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3010 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3015 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3035 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3039 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3043 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3061 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3077 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3079 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3082 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3097 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3099 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3108 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3112 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3130 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3147 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3152 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3164 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3177 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3216 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3241 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3243 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3249 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3257 | -         | -        | -       | X                |
| 59  | MG   | DD    | 301  | -         | -        | -       | X                |
| 59  | MG   | DE    | 302  | -         | -        | -       | X                |

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294559 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 ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1495     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32141 | 14306 | 5964 | 10377 | 1494 |         |         |       |
| 1   | CA    | 1495     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32141 | 14306 | 5964 | 10377 | 1494 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 235      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1901  | 1213 | 342 | 341 | 5 |         |         |       |
| 2   | CB    | 235      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1901  | 1213 | 342 | 341 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AC    | 207      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1613  | 1016 | 315 | 281 | 1 |         |         |       |
| 3   | CC    | 207      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1613  | 1016 | 315 | 281 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 4   | CD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 151      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1147  | 724 | 218 | 201 | 4 |         |         |       |
| 5   | CE    | 151      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1147  | 724 | 218 | 201 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | CF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | CG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | CH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1005  | 636 | 195 | 174 |  |         |         |       |
| 9   | CI    | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1006  | 637 | 195 | 174 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 795   | 499 | 157 | 138 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 795   | 499 | 157 | 138 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | CK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 971   | 611 | 196 | 163 | 1 |         |         |       |
| 12  | CL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 971   | 611 | 196 | 163 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 947   | 585 | 195 | 165 | 2 |         |         |       |
| 13  | CM    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 910   | 564 | 180 | 164 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | AN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | CN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- 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     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 701   | 443 | 140 | 117 | 1 |         |         |       |
| 16  | CP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 701   | 443 | 140 | 117 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 824   | 528 | 152 | 142 | 2 |         |         |       |
| 17  | CQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 824   | 528 | 152 | 142 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |
| 18  | CR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |

- 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       | 1     |
|     |       |          | 630   | 403 | 115 | 110 | 2 |         |         |       |
| 19  | CS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 630   | 403 | 115 | 110 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |
| 20  | CT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | AU    | 25       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 209   | 128 | 51 | 30 |         |         |       |
| 21  | CU    | 25       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 209   | 128 | 51 | 30 |         |         |       |

- Molecule 22 is a RNA chain called RNA (5'-R(\*AP\*AP\*AP\*AP\*AP\*GP\*GP\*AP\*AP\*AP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*CP\*AP\*GP\*UP\*UP\*CP\*AP\*AP\*UP\*CP\*UP\*A)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 22  | AV    | 10       | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 213   | 97 | 42 | 65 | 9 |         |         |       |
| 22  | CV    | 10       | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 213   | 97 | 42 | 65 | 9 |         |         |       |

- Molecule 23 is a RNA chain called tRNA-Gln.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23  | AW    | 75       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1593  | 711 | 281 | 526 | 75 |         |         |       |
| 23  | CW    | 75       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1593  | 711 | 281 | 526 | 75 |         |         |       |

- Molecule 24 is a RNA chain called tRNA-Met.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 24  | AX    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 24  | CX    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |

- Molecule 25 is a RNA chain called tRNA-Gln.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 25  | AY    | 75       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1591  | 711 | 280 | 526 | 74 |         |         |       |
| 25  | CY    | 75       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1591  | 711 | 280 | 526 | 74 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| AY    | 33      | G        | C      | CONFLICT | GB CP001637.1 |
| AY    | 44      | U        | A      | CONFLICT | GB CP001637.1 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| CY    | 33      | G        | C      | CONFLICT | GB CP001637.1 |
| CY    | 44      | U        | A      | CONFLICT | GB CP001637.1 |

- Molecule 26 is a protein called Viomycin.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 26  | AZ    | 6        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 48    | 25 | 13 | 10 |         |         |       |
| 26  | CZ    | 6        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 48    | 25 | 13 | 10 |         |         |       |

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 27  | BA    | 2800     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60311 | 26841 | 11284 | 19387 | 2799 |         |         |       |
| 27  | DA    | 2800     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60313 | 26842 | 11286 | 19386 | 2799 |         |         |       |

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 28  | BB    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2528  | 1126 | 466 | 819 | 117 |         |         |       |
| 28  | DB    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2528  | 1126 | 466 | 819 | 117 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 29  | BC    | 191      | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 1142  | 691 | 221 | 230 |         |         |       |
| 29  | DC    | 191      | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 1142  | 691 | 221 | 230 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 30  | BD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 2105  | 1329 | 417 | 356 | 3 |         |         |       |
| 30  | DD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 2105  | 1329 | 417 | 356 | 3 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1564  | 988 | 300 | 270 | 6 |         |         |       |
| 31  | DE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1564  | 988 | 300 | 270 | 6 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 32  | BF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1624  | 1035 | 304 | 282 | 3 |         |         |       |
| 32  | DF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1624  | 1035 | 304 | 282 | 3 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 33  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BH    | 164      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1252  | 794 | 233 | 224 | 1 |         |         |       |
| 34  | DH    | 160      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1223  | 773 | 229 | 220 | 1 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1042  | 668 | 175 | 198 | 1 |         |         |       |
| 35  | DI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1046  | 670 | 175 | 200 | 1 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L13.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BN    | 139      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1105  | 712 | 207 | 182 | 4 |         |         |       |
| 36  | DN    | 139      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1105  | 712 | 207 | 182 | 4 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 37  | DO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BP    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1114  | 692 | 227 | 193 | 2 |         |         |       |
| 38  | DP    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1114  | 692 | 227 | 193 | 2 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 39  | DQ    | 139      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1107  | 707 | 209 | 184 | 7 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 40  | BR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |
| 40  | DR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 41  | BS    | 99       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 771   | 486 | 155 | 130 |  |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 41  | DS    | 101      | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 777   | 489 | 156 | 132 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BT    | 138      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1142  | 710 | 235 | 196 | 1 |         |         |       |
| 42  | DT    | 138      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1142  | 710 | 235 | 196 | 1 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 604 | 202 | 151 | 1 |         |         |       |
| 43  | DU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 604 | 202 | 151 | 1 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 44  | DV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |
| 45  | DW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 46  | BX    | 93       | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 726   | 471 | 132 | 123 |         |         |       |
| 46  | DX    | 93       | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 726   | 471 | 132 | 123 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BY    | 101      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 776   | 500 | 149 | 123 | 4 |         |         |       |
| 47  | DY    | 101      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 776   | 500 | 149 | 123 | 4 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | BZ    | 177      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1404  | 897 | 253 | 252 | 2 |         |         |       |
| 48  | DZ    | 177      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1404  | 897 | 253 | 252 | 2 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | B0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |
| 49  | D0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | B1    | 94       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 715   | 448 | 141 | 125 | 1 |         |         |       |
| 50  | D1    | 94       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 732   | 460 | 146 | 125 | 1 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51  | B2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |
| 51  | D2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B3    | 60       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 468   | 298 | 91 | 78 | 1 |         |         |       |
| 52  | D3    | 60       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 468   | 298 | 91 | 78 | 1 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | B4    | 31       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 226   | 142 | 37 | 43 | 4 |         |         |       |
| 53  | D4    | 31       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 226   | 142 | 37 | 43 | 4 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54  | B5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 54  | D5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55  | B6    | 51       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 411   | 253 | 84 | 70 | 4 |         |         |       |
| 55  | D6    | 46       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 390   | 241 | 80 | 65 | 4 |         |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 56  | B7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 419   | 257 | 105 | 55 | 2 |         |         |       |
| 56  | D7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 419   | 257 | 105 | 55 | 2 |         |         |       |

- Molecule 57 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 57  | B8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 508   | 326 | 102 | 78 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 57  | D8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 508   | 326 | 102 | 78 | 2 |         |         |       |

- Molecule 58 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 58  | B9    | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 299   | 183 | 67 | 46 | 3 |         |         |       |
| 58  | D9    | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 299   | 183 | 67 | 46 | 3 |         |         |       |

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 59  | BA    | 400      | Total | Mg  | 0       | 0       |
|     |       |          | 400   | 400 |         |         |
| 59  | AK    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 59  | DF    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | CV    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 59  | BE    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AW    | 7        | Total | Mg  | 0       | 0       |
|     |       |          | 7     | 7   |         |         |
| 59  | BP    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AX    | 7        | Total | Mg  | 0       | 0       |
|     |       |          | 7     | 7   |         |         |
| 59  | DR    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | CA    | 92       | Total | Mg  | 0       | 0       |
|     |       |          | 92    | 92  |         |         |
| 59  | B5    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | BB    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | D6    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AE    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 59  | BF    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | BX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | AA    | 133      | Total<br>133 | Mg<br>133 | 0       | 0       |
| 59  | BQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | CQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | CX    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | BU    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | AD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | BN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | BY    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | BR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | DA    | 275      | Total<br>275 | Mg<br>275 | 0       | 0       |
| 59  | CE    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | DD    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | AL    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | DE    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | AH    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | BZ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | DZ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | AC    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | DB    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59  | D5    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 59  | BD    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 59  | AT    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 59  | B0    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 59  | AO    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 59  | AY    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 59  | AF    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 59  | BH    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

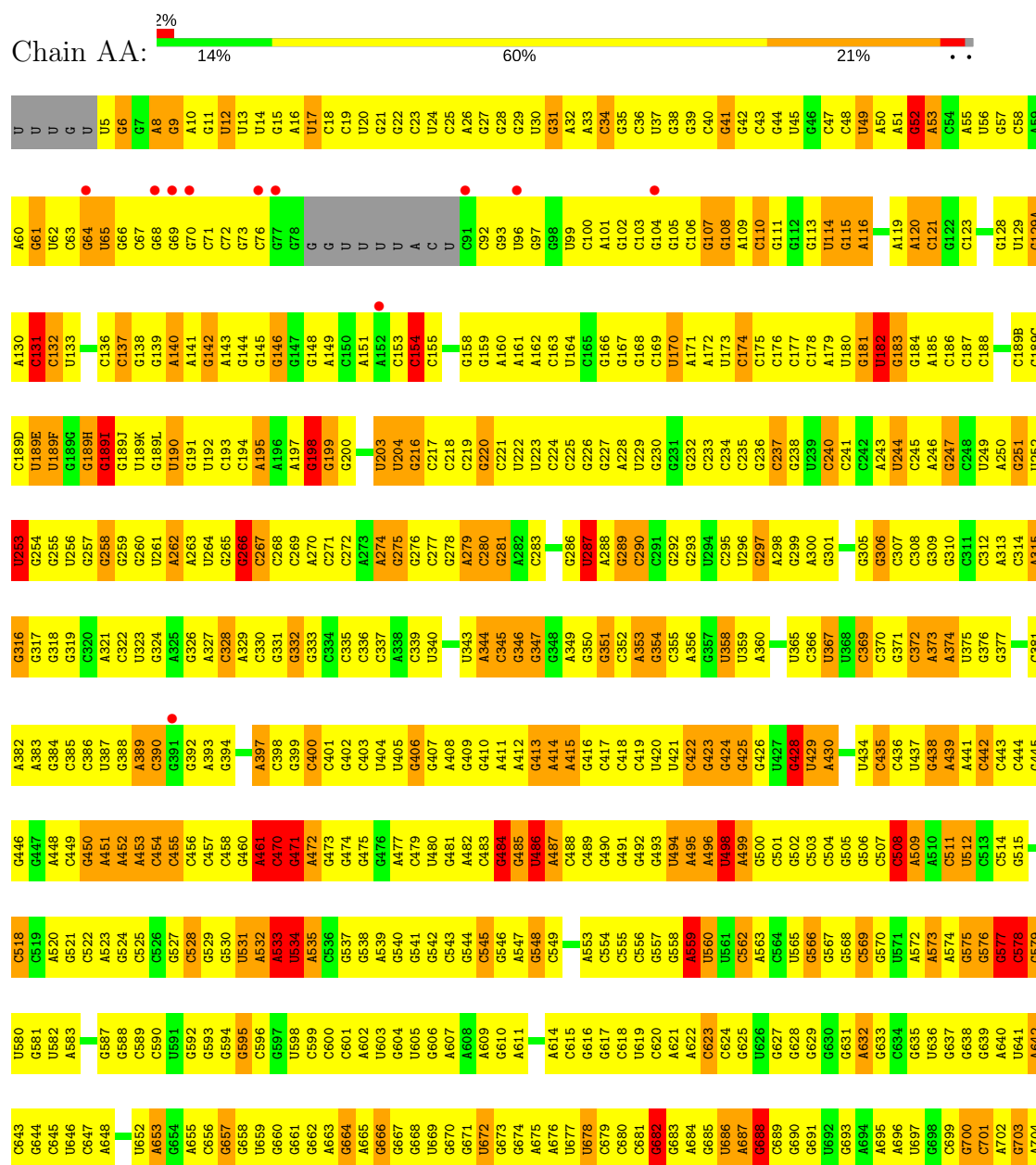
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 60  | B5    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 60  | B4    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 60  | AD    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 60  | B9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 60  | D9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 60  | D5    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 60  | D4    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 60  | CD    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

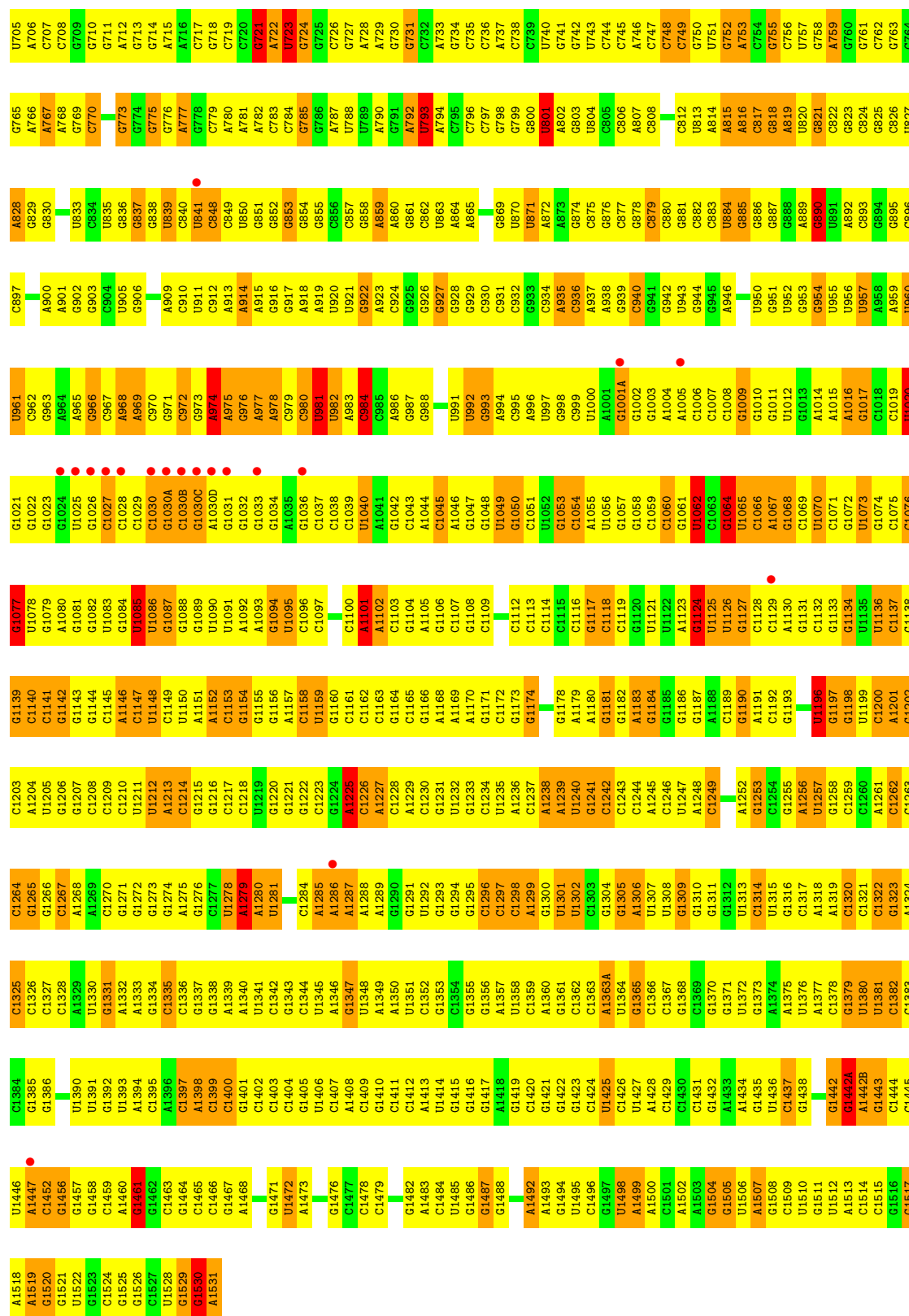
### 3 Residue-property plots

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 ribosomal RNA

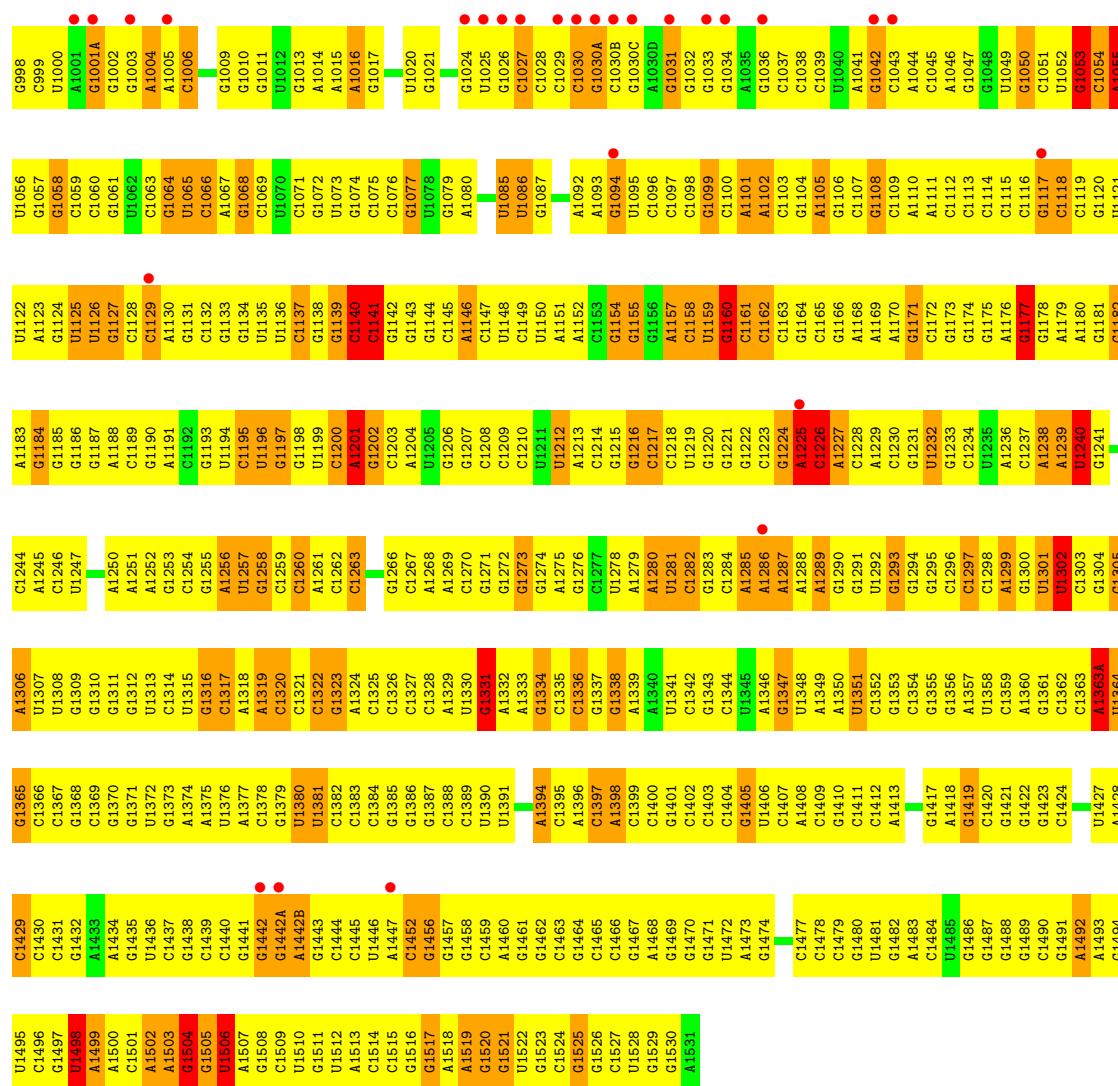




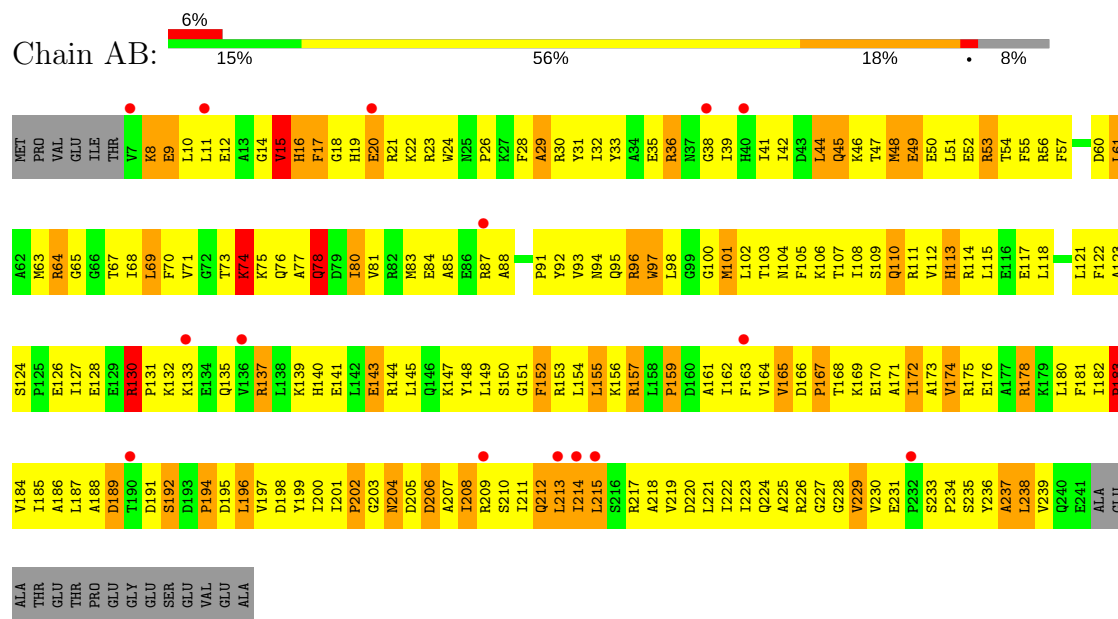


• Molecule 1: 16S ribosomal RNA

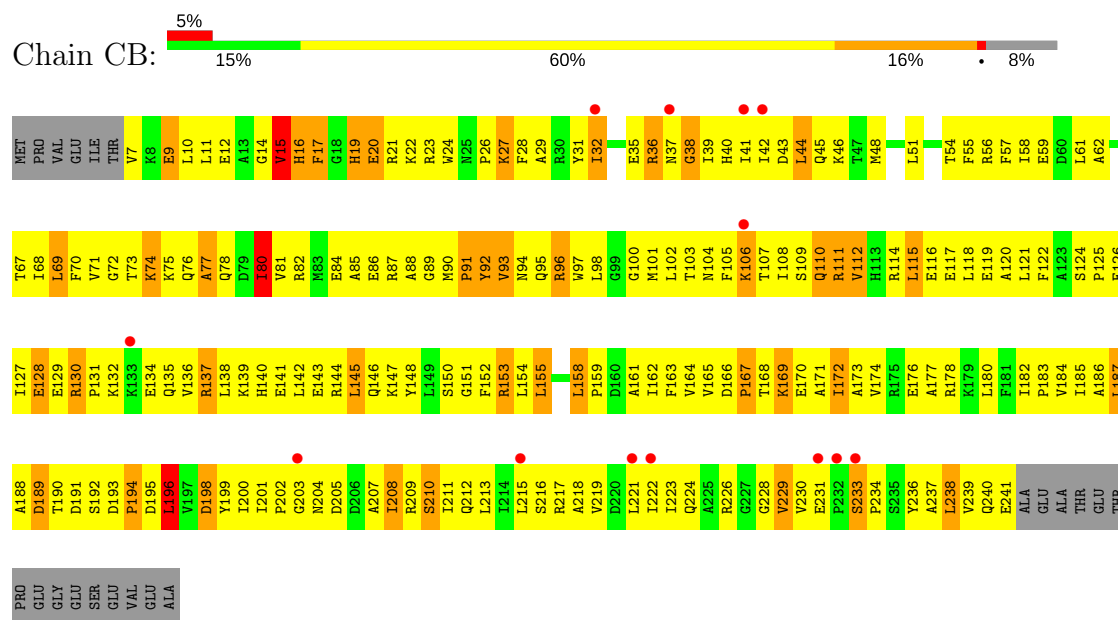
|      |      |      |      |      |      |      |      |      |      |      |      |       |       |     |
|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-----|
| A938 | C875 | G809 | C748 | G688 | G627 | A563 | C503 | A430 | C370 | G309 | C247 | C188  | G127  | U   |
| G939 | G876 | C810 | C749 | C689 | G628 | C564 | C504 | A431 | G371 | G310 | C246 | G189  | G128  | U   |
| C940 | C877 | C811 | G750 | G690 | G629 | U565 | G505 | A432 | C372 | C311 | U249 | C189A | U129  | U   |
| G941 | C878 | C812 | U751 | G691 | G630 | G566 | G506 | C433 | A373 | C312 | A250 | C189B | G129A | U   |
| G942 | C879 | U813 | G752 | U692 | G631 | G567 | C507 | U434 | A374 | G313 | G251 | C189C | G64   | U   |
| U943 | C880 | A814 | G753 | G693 | A632 | G568 | C508 | C435 | U375 | U65  | U252 | C189D | C131  | U5  |
| G944 | C881 | A815 | C754 | A694 | G633 | C569 | A509 | U436 | G376 | G316 | U253 | U189E | C132  | G6  |
| G945 | C882 | A816 | G755 | A695 | G634 | G570 | A510 | U437 | G377 | G317 | G254 | U189F | C133  | G7  |
| A946 | C883 | C817 | G756 | A696 | G635 | U571 | C511 | U438 | G378 | A8   | G255 | U189G | C134  | A8  |
| G947 | U884 | U818 | U757 | U697 | U636 | A573 | C512 | U439 | C379 | G318 | U256 | G189H | C135  | G9  |
| C948 | C885 | A819 | G758 | G698 | G637 | A574 | C513 | A441 | G380 | C320 | G257 | G189I | C136  | A10 |
| A949 | G886 | U820 | A759 | G699 | G638 | A575 | C514 | C442 | C381 | A321 | G258 | G189J | C137  | G11 |
| U950 |      | G821 | G760 | G700 | G639 | A576 | C515 | C443 | A382 | C322 | G259 | U189K | G138  | U12 |
| G951 | A889 | C822 | G761 | C701 | A640 | C576 | C516 | C444 | A383 | U323 | G260 | G189L | G139  | U13 |
| U952 | G890 | G823 | C762 | A702 | U641 | G577 | C517 | G445 | G384 | G324 | U261 | U190  | A140  | U14 |
| G953 | U891 | C824 | G763 | G703 | A642 | C578 | C518 | G446 | C385 | A325 | A262 | G191  | A141  | G15 |
| G954 | A892 | G825 | C764 | A704 | G643 | G579 | C519 | G447 | U386 | G326 | A263 | U192  | G142  | A16 |
| U955 | C893 | C826 | G765 | U705 | G644 | U580 | A520 |      | U387 | A327 | U264 | C193  | G143  | U17 |
| U956 | G894 | U827 | A766 | A706 | C545 | G581 | G521 | G450 | G388 | C328 | G265 | C194  | G144  | C18 |
| U957 | G895 | A828 | A767 | C707 | U646 | U582 | C522 | A451 | A389 | A329 | G266 | A195  | G145  | C19 |
| A958 | C896 | G829 | A768 | C708 | C647 | A583 | A523 | A452 | C390 | C330 | C267 | A196  | G146  | U20 |
| A959 | C897 | G830 | G769 | G709 | A648 | G584 | G524 | A453 | G391 | G331 | C268 | U197  | G147  | U21 |
| U960 | G898 | U831 | C770 | G710 | G649 | G585 | C525 | C454 | G392 | G332 | C269 | G198  | G148  | G22 |
| U961 | C899 | C832 | G771 | U711 | G650 | C586 | C526 | C455 | A393 | G333 | A270 | G199  |       | G23 |
| C962 | A900 | U833 | U772 | A712 | C651 | G587 | G527 | C456 | G394 | C334 | C271 | G200  | A     | C24 |
| G963 | A901 | C834 | G773 | G713 | U652 | C528 | C528 | C457 | C395 | C335 | C272 | C201  | A152  | C25 |
| A964 | G902 | U835 | G774 | G714 | A653 | G529 | G529 | A458 | G396 | C336 | A273 | U202  | A153  | A26 |
| A965 | C903 | G836 | G775 | A715 | G654 | U591 | G530 | G460 | A397 | C337 | A274 | U203  | C154  | G27 |
| G966 | C904 | G837 | G776 | A716 | A655 | G592 | U531 | G461 | C398 | A338 | G275 | U204  | C155  | G28 |
| C967 | U905 | U838 | A777 | C717 | G657 | G593 | A532 | C470 | G399 | C339 | G276 | G216  | G156  | G29 |
| A968 |      | U839 | G778 | G718 | G658 | G594 | A533 | G471 | C400 | U340 | C277 | C217  | G157  | U30 |
| A969 |      | C840 | C779 | C719 | U659 | G595 | U534 | A472 | C401 | C341 | U278 | C218  | G158  | G31 |
| C970 | A908 | U841 | A780 | C720 | G660 | C596 | A535 | G473 | G402 | C342 | A279 | C219  | U99   | A32 |
| G971 | C910 | C848 | A781 | G721 | G661 | C597 | C536 | G474 | C403 | U343 | C281 | C220  | C100  | A33 |
| C972 |      | G849 | G782 | A722 | G662 | U598 | G537 | G475 | U404 | A344 | A282 | C221  | A101  | C34 |
| G973 | A913 | U850 | C783 | U723 | A663 | C599 | G538 | G476 | U405 | C345 | C283 | U222  | G102  | C35 |
| A974 | A914 | G851 | G784 | G724 | G664 | C600 | A539 | A477 | G406 | G346 | G284 | U223  | C103  | C36 |
| A975 | A915 | G852 |      | G725 | A665 | C601 | G540 | C479 | G407 | G347 | G285 | C224  | G104  | U37 |
| G976 | G916 | G853 | A787 | C726 | G666 | A602 | G541 | U480 | A408 | G348 | G286 | C225  | G105  | G38 |
| A977 | C917 | G854 | U788 | G727 | G667 | U603 | G542 | G481 | G409 | A349 | U287 | G227  | C106  | G39 |
| C978 | A918 | G855 | U789 | A728 | G668 | G604 | C543 | A482 | C410 | G350 | A288 | G107  | G107  | C40 |
| A979 | A919 | C856 | A790 | U729 | U669 | U605 | G544 | C483 | A411 | C352 | G289 | U229  | A109  | G42 |
| C980 | U920 | C857 | G791 | G730 | G670 | G606 | C545 | G484 | A412 | C353 | C290 | G230  | C110  | G43 |
| U981 | U921 | G858 | A792 | G731 | G671 | A607 | G546 | G485 | G413 | A354 | C291 | G231  | A171  | C44 |
| U982 | G922 | A859 | U793 | C732 | U672 | A608 | A547 | U486 | A414 | G355 | G292 | G232  | G111  | G45 |
| A983 | A923 | A860 | A794 | A733 | G673 | A609 | G548 | A487 | A415 | C356 | G293 | C233  | C174  | U46 |
| C984 | C924 | G861 | C795 | G734 | G674 | G610 | C549 | C488 | G416 | A357 | C294 | C234  | C175  | G46 |
| C985 | G925 | C862 | C796 | C735 | A675 | A611 | G550 | C489 | C417 | G357 | U358 | C235  | C176  | C47 |
| A986 | G926 | U863 | C797 | C736 | A676 | G612 | U551 | G490 | C418 | U359 | G297 | C236  | C177  | C48 |
| G987 | G927 | A864 | A797 | A737 | U677 | C613 | U552 | G491 | C419 | A360 | A298 | G237  | C178  | U49 |
| G988 | G928 | A865 | G799 | C738 | U678 | A614 | A553 | G492 | U420 | G361 | G299 | G238  | G117  | A50 |
| C989 | G929 | C866 | G800 | C739 | C679 |      | C554 | G493 | U421 | A362 | G300 | G239  | U118  | A51 |
| C990 | C930 | G867 | U801 | U740 | C680 | U619 | C555 | U494 | C422 | G363 | A300 | U180  | U180  | G52 |
| U991 | C931 | C868 | A802 | G741 | C681 | C620 | C556 | A495 | G423 | A364 | G301 | C240  | A120  | A53 |
| U992 | C932 | G869 | G803 | G742 | G682 | A621 | G557 | A496 | G424 | A365 | G302 | C241  | G121  | C54 |
| C993 | G933 | U870 | U804 | U743 | G683 | A622 | G558 | U498 | G425 | U365 | A303 | C242  | G122  | A55 |
| A994 | C934 | U871 | C805 | C744 | A684 | C623 | A559 | A499 | G426 | C366 | U304 | A243  | G183  | U56 |
| C995 | A935 | A872 | C906 | C745 | G685 | C624 | U560 | G500 | U427 | U367 | G305 | U244  | A185  | G57 |
| A996 | C936 | A873 | A807 | U746 | U686 | G625 | U561 | C501 | G428 | U368 | G306 | C245  | C186  | C58 |
| U997 | A937 | C874 | C808 | C747 | A887 | U626 | C562 | G502 | U429 | C369 |      | A246  | G126  | A59 |



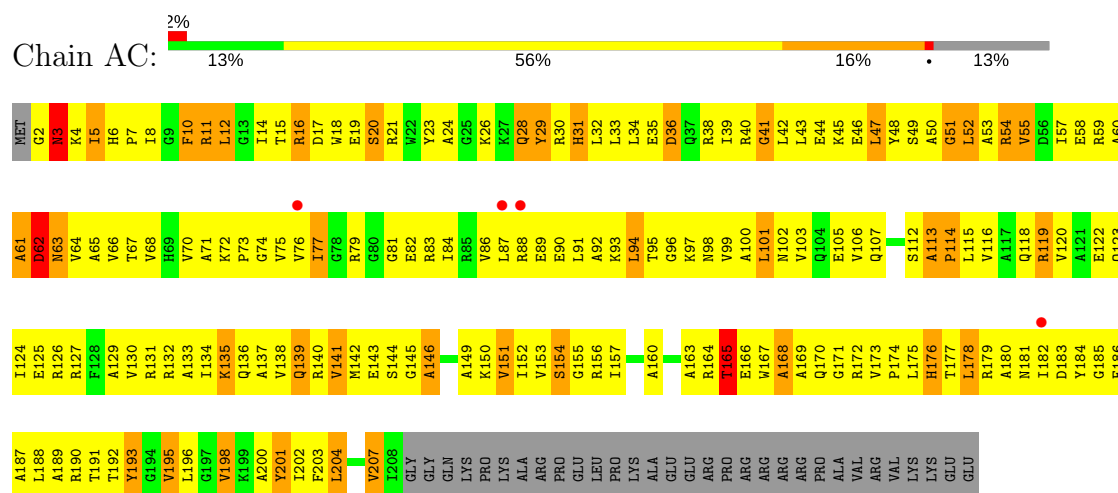
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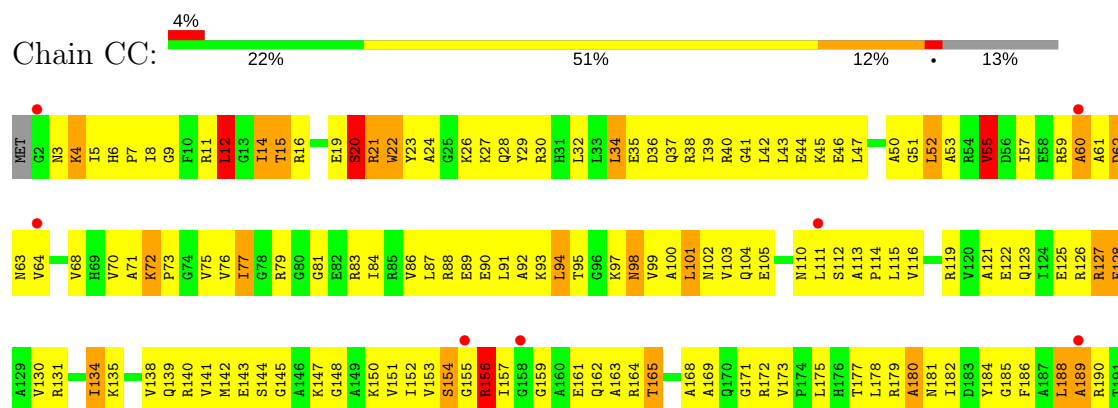
• Molecule 2: 30S ribosomal protein S2



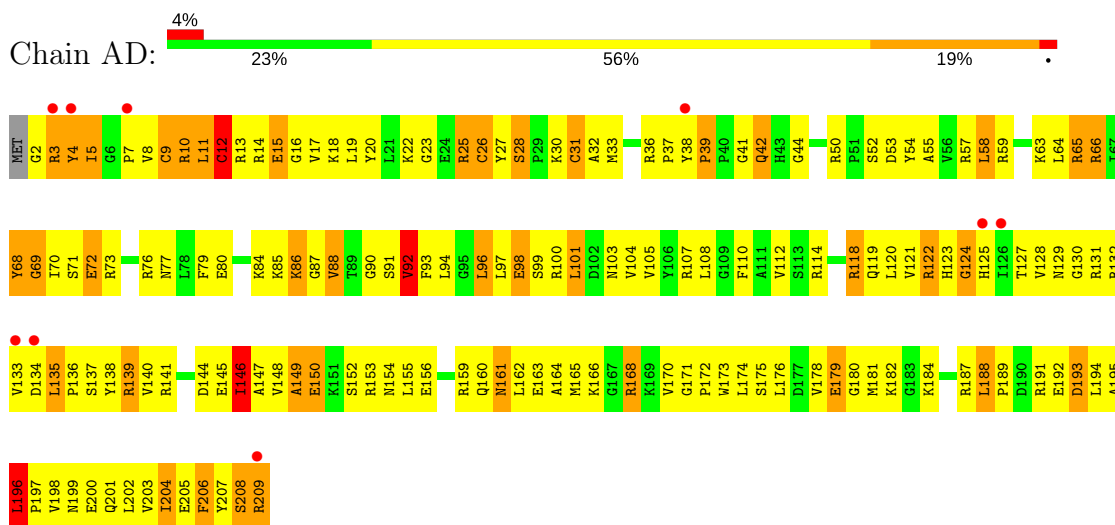
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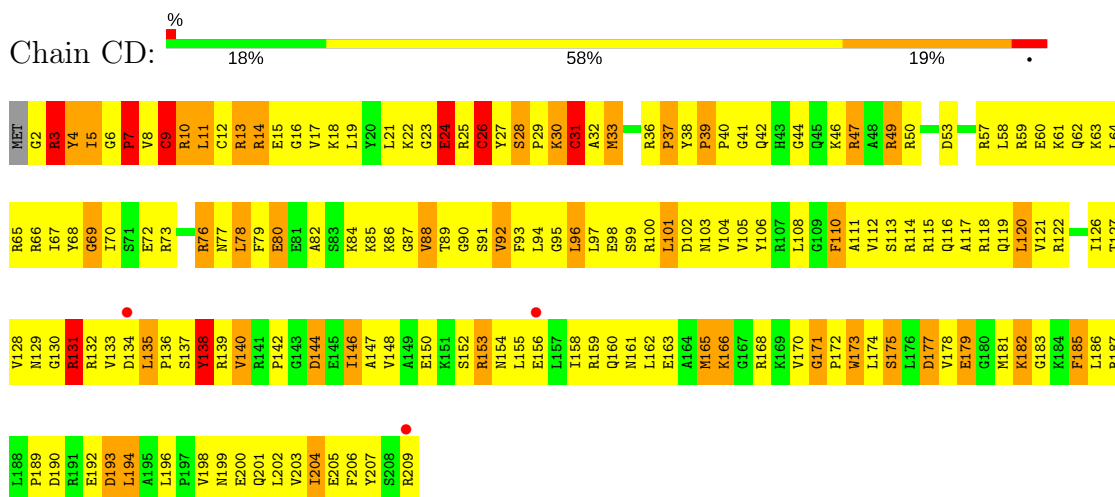
• Molecule 3: 30S ribosomal protein S3



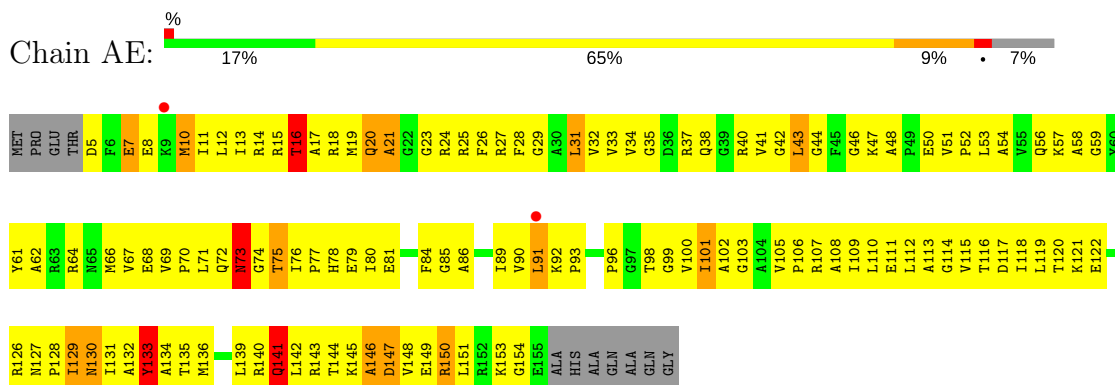
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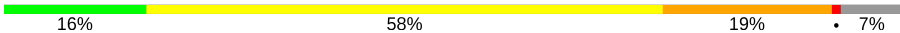
- Molecule 4: 30S ribosomal protein S4

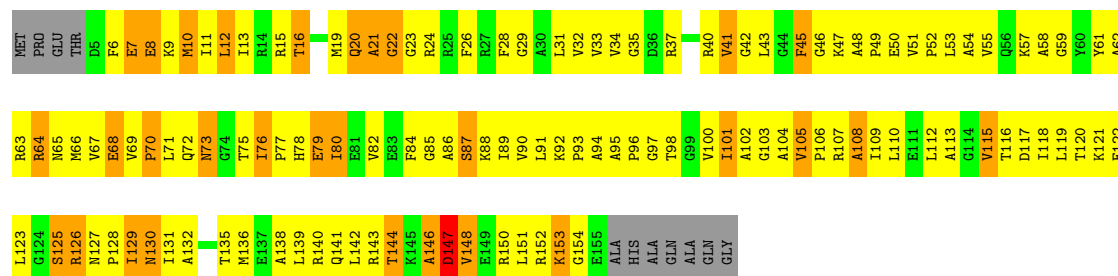


- Molecule 5: 30S ribosomal protein S5



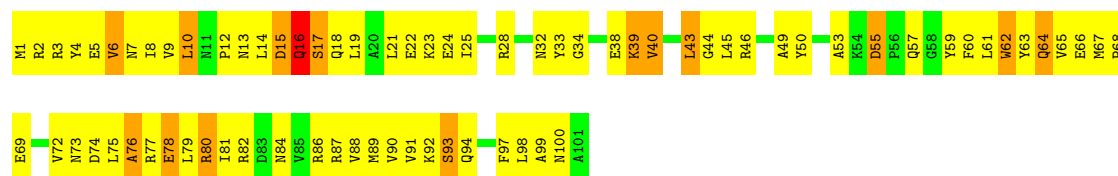
- Molecule 5: 30S ribosomal protein S5

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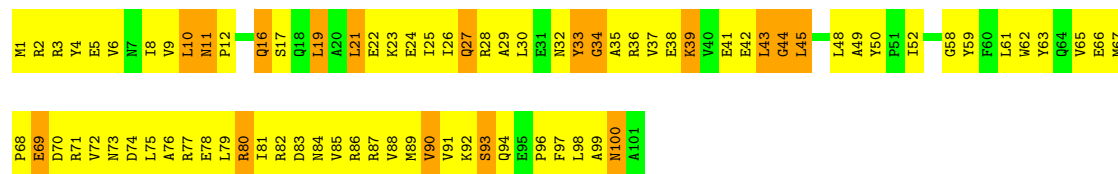
- Molecule 6: 30S ribosomal protein S6

Chain AF: 



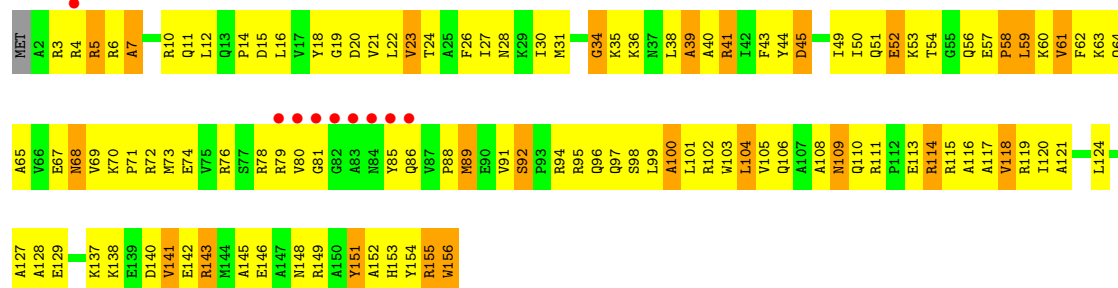
- Molecule 6: 30S ribosomal protein S6

Chain CF: 



- Molecule 7: 30S ribosomal protein S7

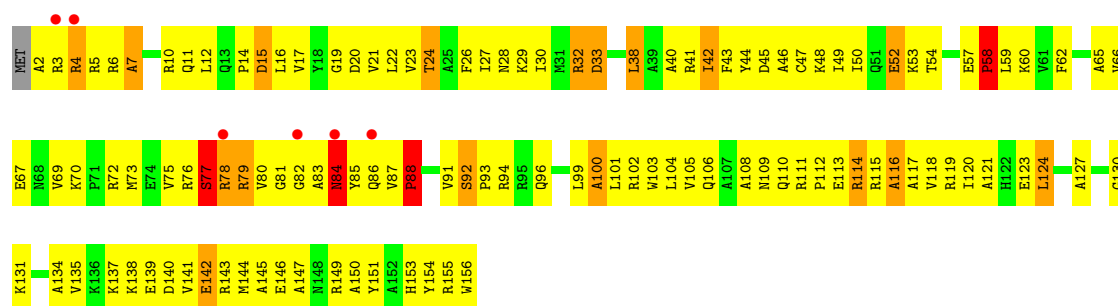
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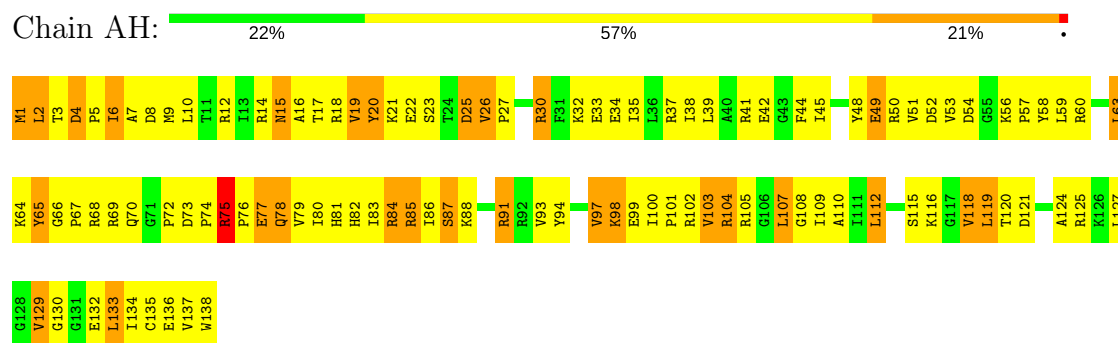
- Molecule 7: 30S ribosomal protein S7

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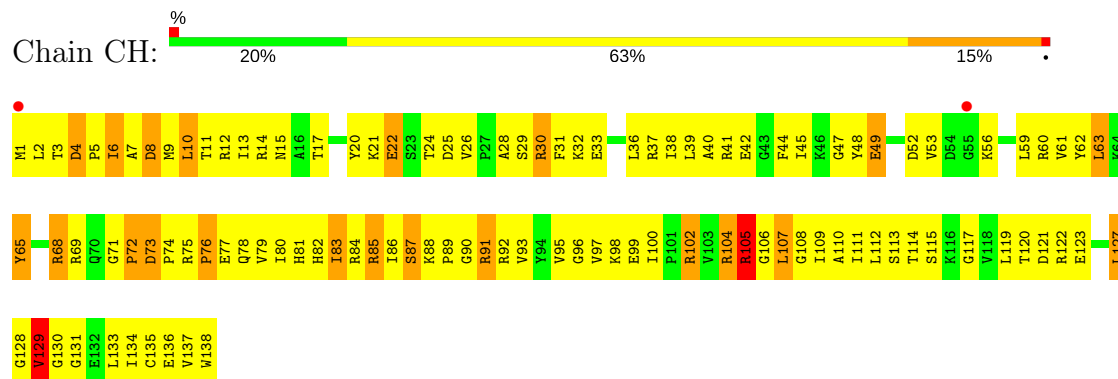




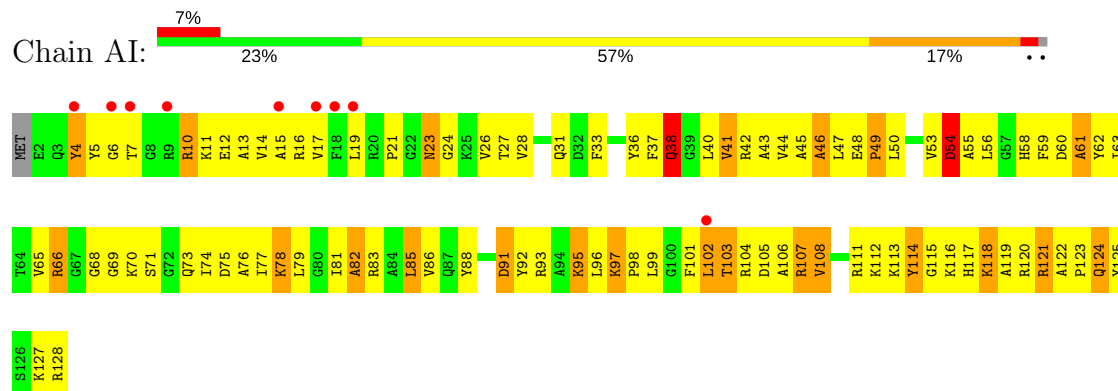
- Molecule 8: 30S ribosomal protein S8



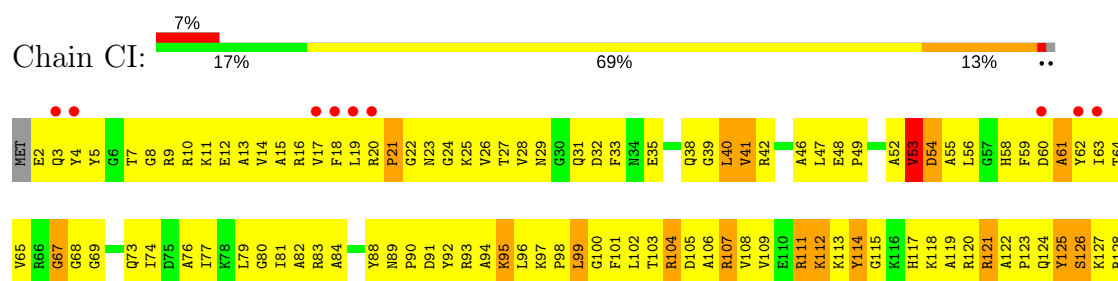
- Molecule 8: 30S ribosomal protein S8



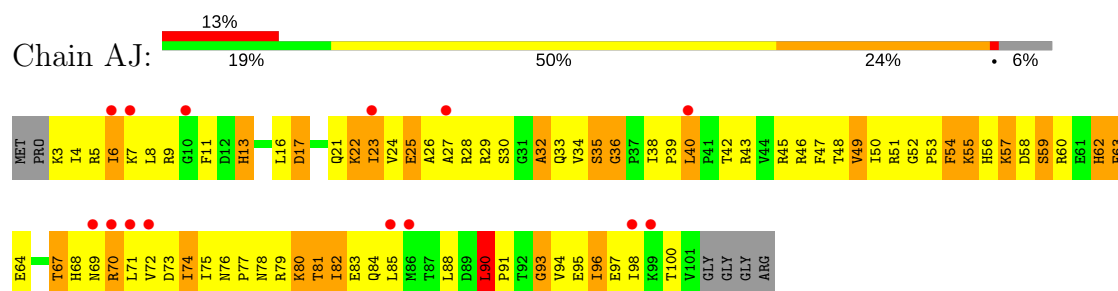
- Molecule 9: 30S ribosomal protein S9



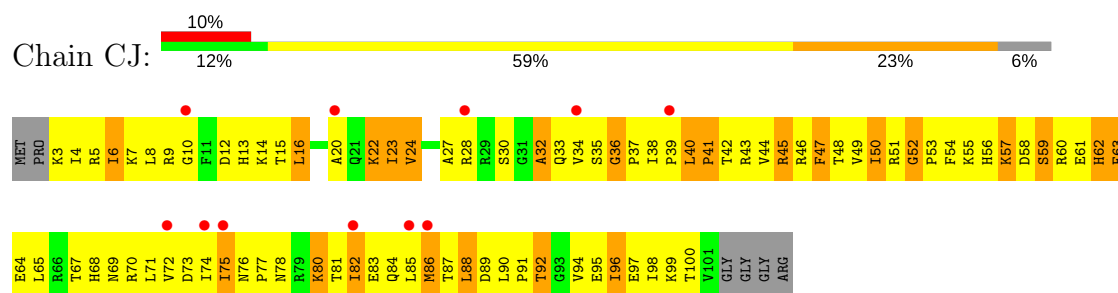
- Molecule 9: 30S ribosomal protein S9



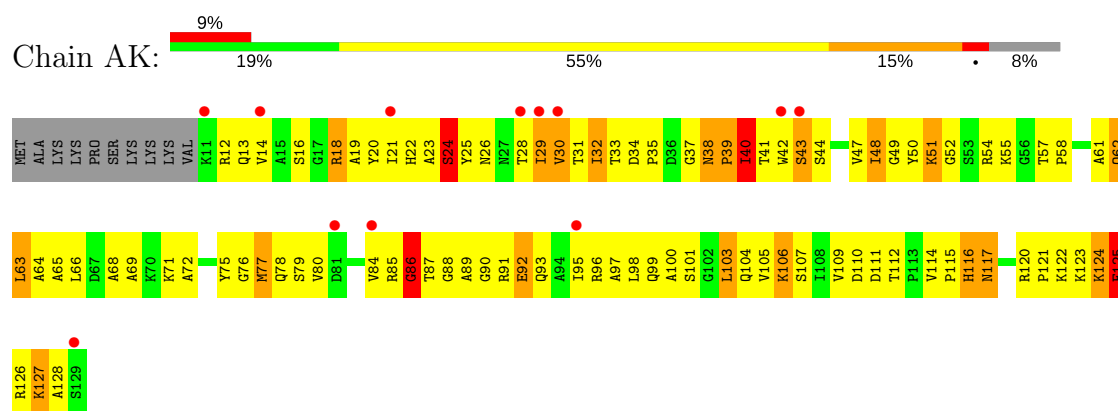
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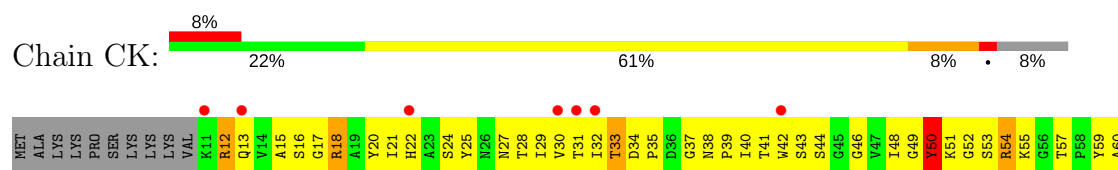
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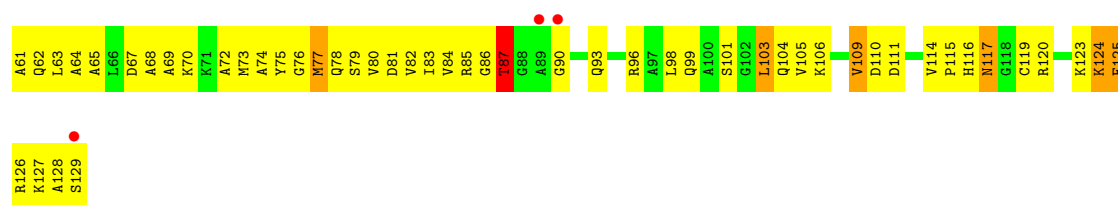
• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11







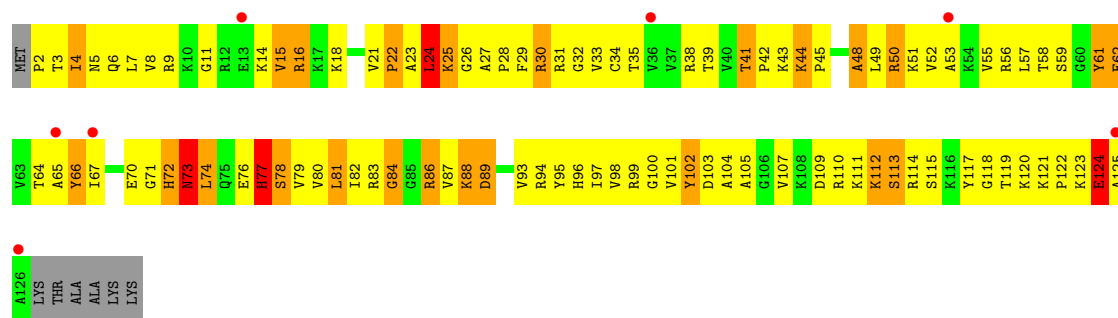
- Molecule 12: 30S ribosomal protein S12

Chain AL: 19% 54% 20% 5%



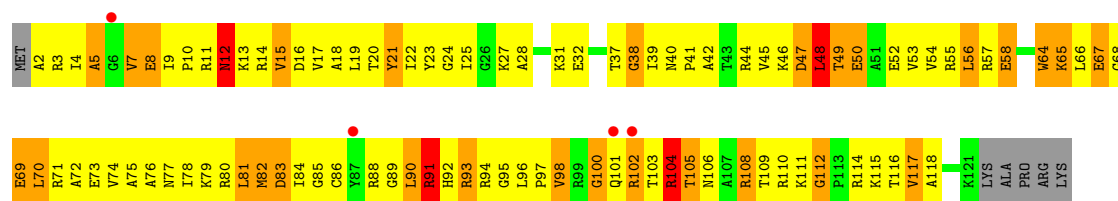
- Molecule 12: 30S ribosomal protein S12

Chain CL: 19% 55% 18% 5%



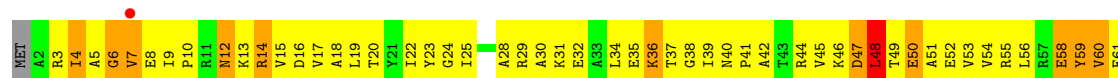
- Molecule 13: 30S ribosomal protein S13

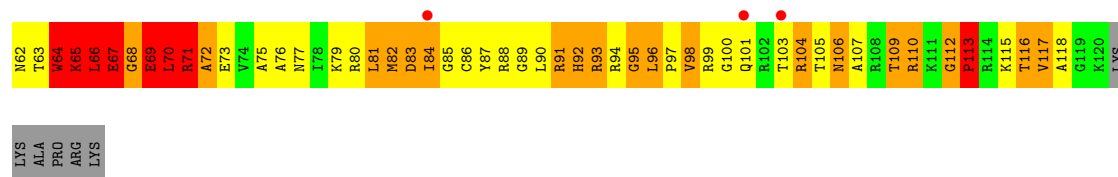
Chain AM: 17% 52% 22% 5%



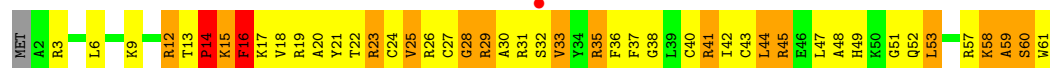
- Molecule 13: 30S ribosomal protein S13

Chain CM: 13% 51% 24% 7% 6%

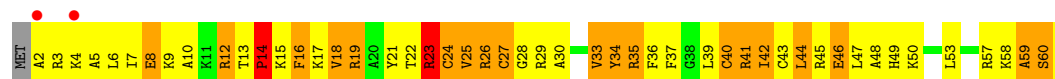
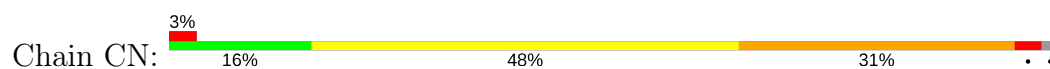




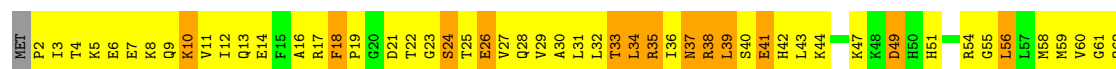
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

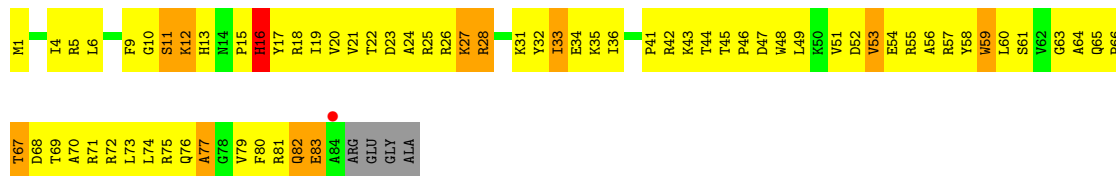


- Molecule 16: 30S ribosomal protein S16



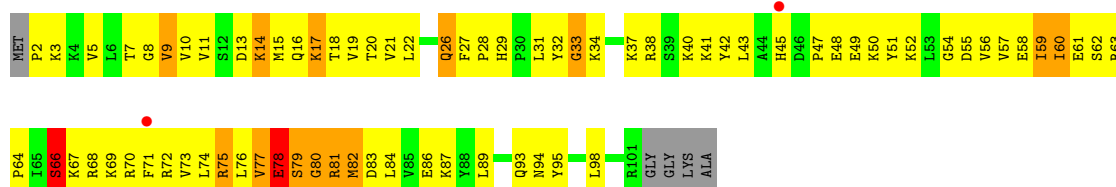
- Molecule 16: 30S ribosomal protein S16

Chain CP: 



- Molecule 17: 30S ribosomal protein S17

Chain AQ: 



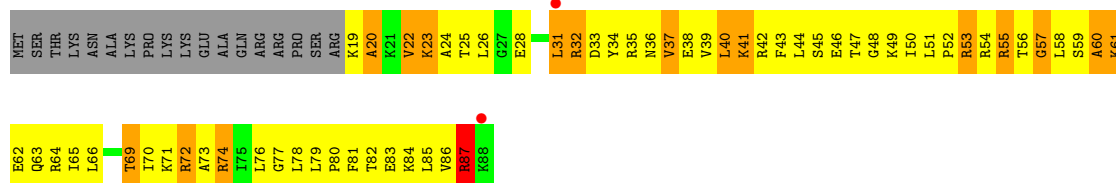
- Molecule 17: 30S ribosomal protein S17

Chain CQ: 



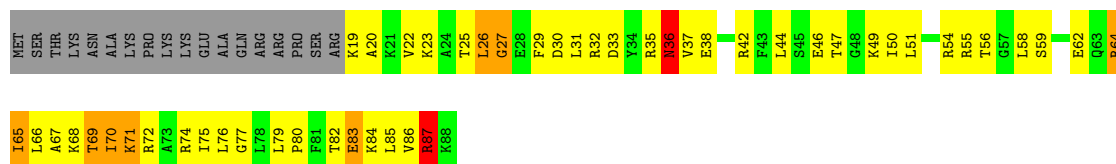
- Molecule 18: 30S ribosomal protein S18

Chain AR: 

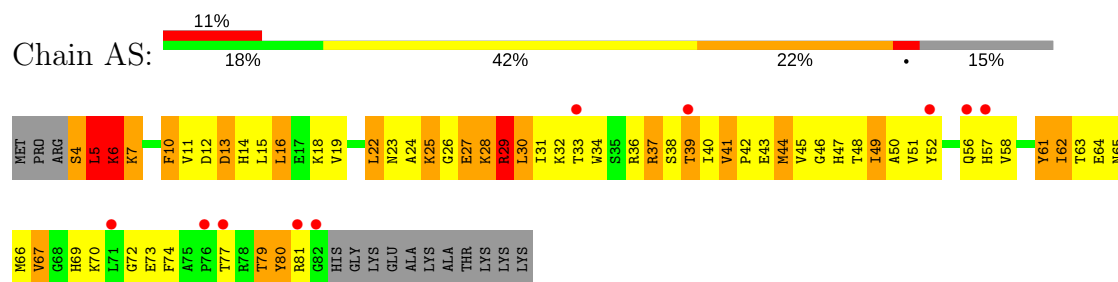


- Molecule 18: 30S ribosomal protein S18

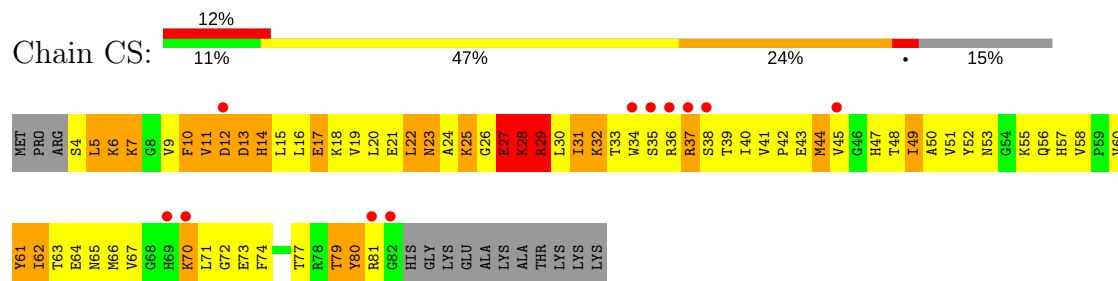
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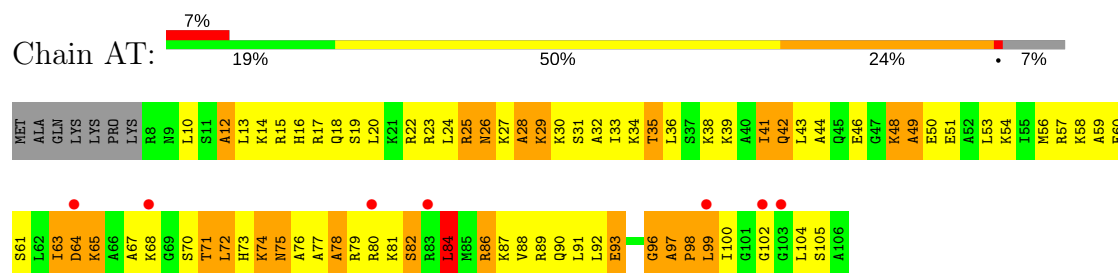
- Molecule 19: 30S ribosomal protein S19



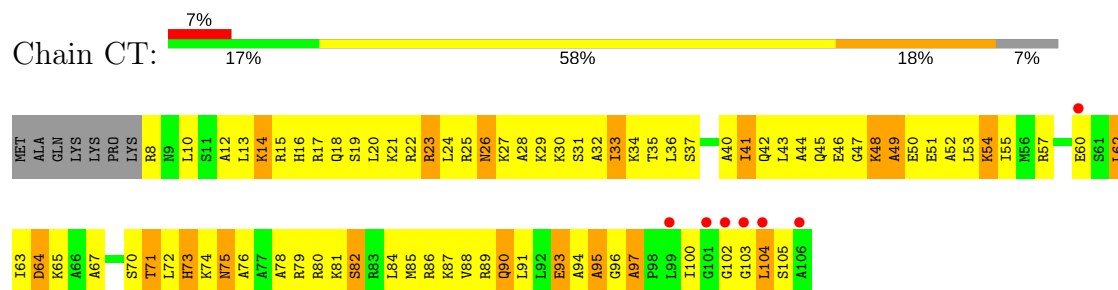
- Molecule 19: 30S ribosomal protein S19



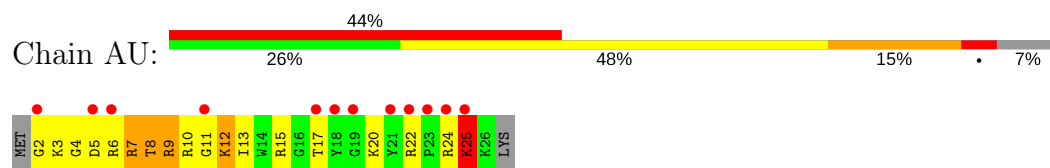
- Molecule 20: 30S ribosomal protein S20



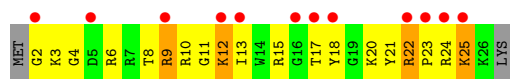
- Molecule 20: 30S ribosomal protein S20



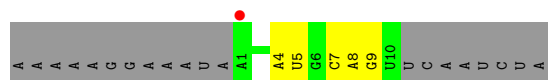
- Molecule 21: 30S ribosomal protein Thx



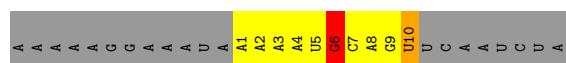
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: RNA (5'-R(\*AP\*AP\*AP\*AP\*AP\*GP\*GP\*AP\*AP\*AP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*CP\*AP\*GP\*UP\*UP\*CP\*AP\*AP\*UP\*CP\*UP\*A)-3')



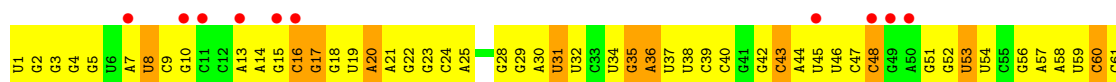
- Molecule 22: RNA (5'-R(\*AP\*AP\*AP\*AP\*AP\*GP\*GP\*AP\*AP\*AP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*CP\*AP\*GP\*UP\*UP\*CP\*AP\*AP\*UP\*CP\*UP\*A)-3')



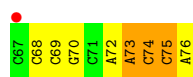
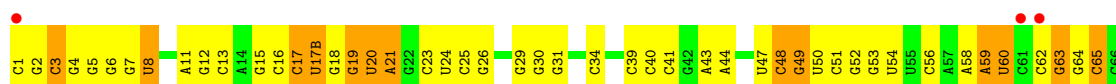
- Molecule 23: tRNA-Gln



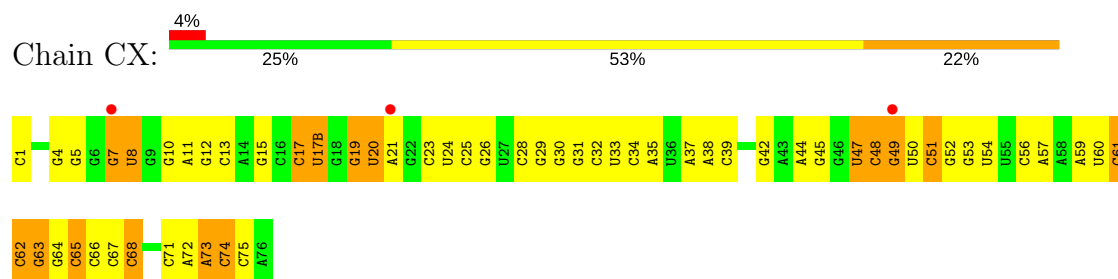
- Molecule 23: tRNA-Gln



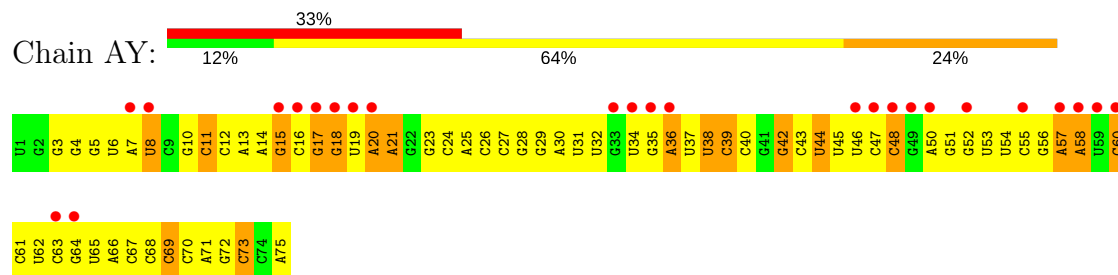
- Molecule 24: tRNA-Met



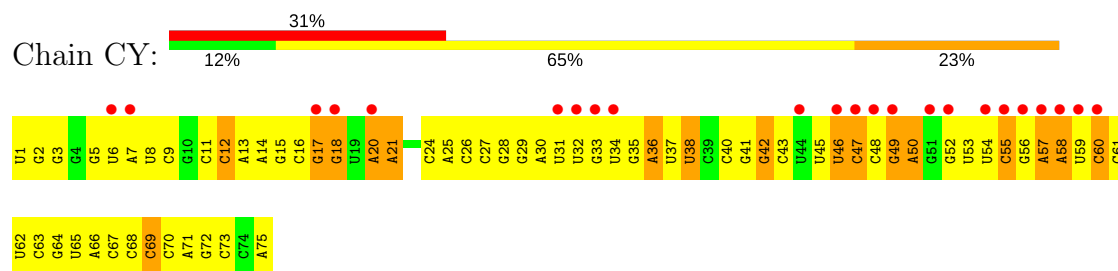
- Molecule 24: tRNA-Met



- Molecule 25: tRNA-Gln



- Molecule 25: tRNA-Gln



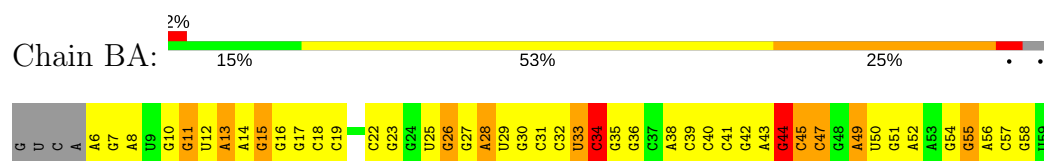
- Molecule 26: Viomycin



- Molecule 26: Viomycin



- Molecule 27: 23S ribosomal RNA



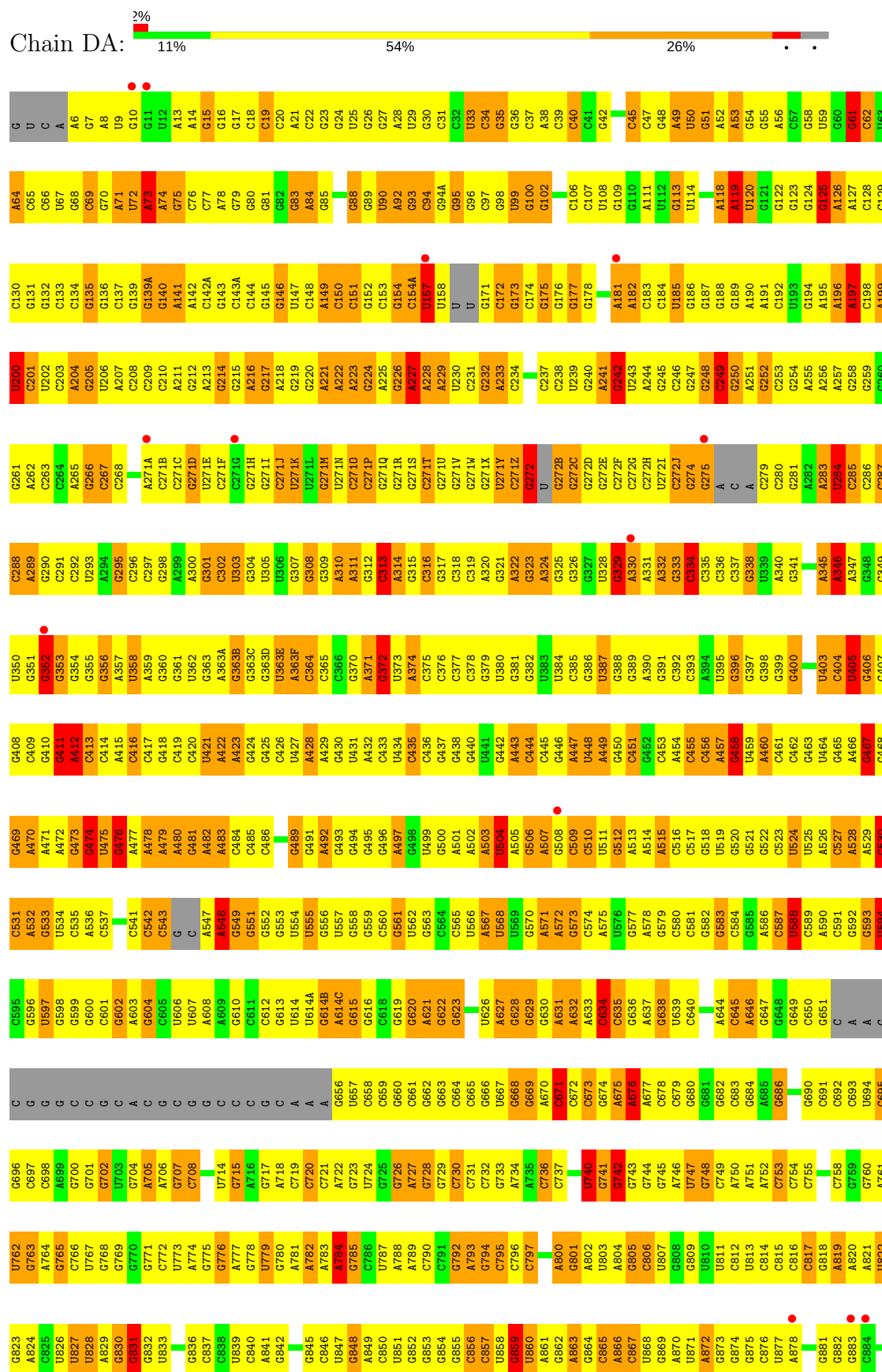


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| C1924 | A1854 | C1790 | C1710  | G1649 | A1587  | G1520  | C1398  | G1334 | G1209  | C1145 | U     | U1019 |
| C1925 | G1855 | C1711 | C1711  | G1650 | C1458  | U1523  | G1399  | U1335 | A1210  | C1146 | U     | A1020 |
| C1926 | G1856 | C1712 | C1712  | G1651 | C1459  | G1524  | G1400  | G1336 | U1211  | A1217 | A     | A1021 |
| A1927 | G1857 | U1794 | U1713  | A1652 | G1591  | G1525  | C1403  | G1337 | A1212  | A1274 | A     | G1022 |
| A1928 | G1858 | C1795 | G1714  | G1653 | A1460  | G1526  | C1402  | G1338 | A1213  | A1275 | A     | U1023 |
| G1929 | A1859 | U1796 | G1717  | A1654 | C1462  | G1527  | C1403  | G1339 | A1214  | A1276 | A     | G1024 |
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| G1933 | G1863 | C1800 | G1721  | C1658 | G1466  | C      | C1407  | G1345 | C1218  | G1280 | G     | A1028 |
| U1934 | U1864 | U1739 | U1739  | U1659 | C1467  | C      | C1408  | C1346 | G1219  | G1281 | C     | A1029 |
| G1935 | G1865 | A1802 | G1740  | C1660 | C1468  | C      | C1409  | C1347 | A1220  | U1282 | G     | G1030 |
| A1936 | C1866 | A1803 | A1741  | G1661 | A1469  | G      | G1410  | G1348 | C1221  | G1283 | U     | G1031 |
| A1937 | A1876 | C1804 | G1742  | C1662 | G1470  | U      | C1411  | A1349 | C1221A | A1284 | A     | A1032 |
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| U1939 | A1878 | C1806 | C1604  | C1604 | A1472  | C      | G1413  | U1352 | G1223  | A1286 | U     | G1034 |
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| G1956 | C1894 | G1823 | A1759  | G1681 | G1620  | C1552  | G1430  | G1367 | A1241  | C1180 | G1114 | A1054 |
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|       |       | A1904 |        | A1630 | U1629  | A1562  | C1439  | U1378 | C1250  | A1189 |       | G     |
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|       |       | A1913 | U1779  | G1699 | A1637  | A1570  | C1446  | G1386 |        | C1135 |       | G     |
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|       |       | A1916 | G1783  | G1703 | A1642  | A1509B | G1450  | G1389 |        | G1138 |       | G     |
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|       |       | U1919 | U1787  | G1707 | A1646  | A1582  | U1453  | A1393 | A1268  | U1205 |       | U     |
|       |       | C1982 |        |       |        | A1583  | U1454  |       | A1269  | A1142 |       | C     |
|       |       | G1983 |        |       |        | C1584  | U1455  |       |        | A1143 |       | C     |
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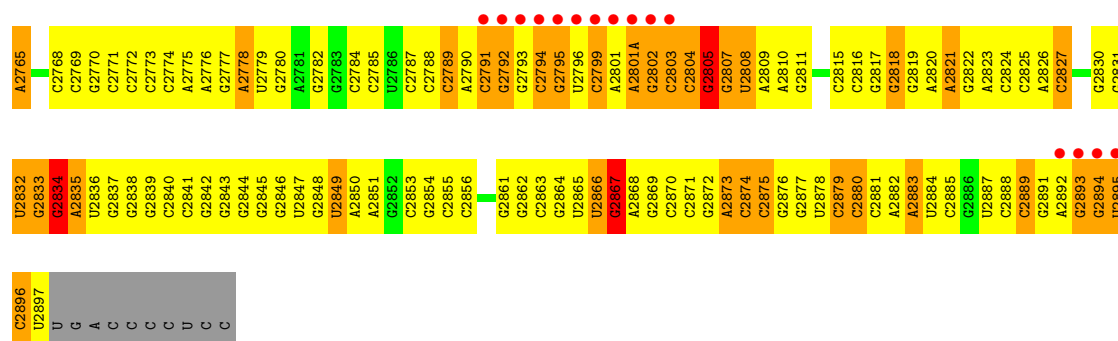
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| G2872 | G2811 | G2747  | U2687 | C2560 | C2622 | C2560 | C2498 | U2437 | G2375 | G2251 |       | C2116 | A2054 | U1991 |
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## ● Molecule 27: 23S ribosomal RNA

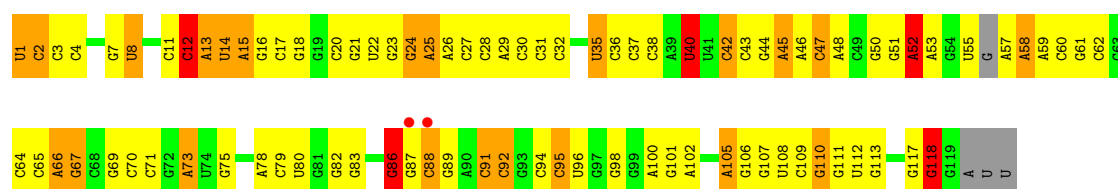




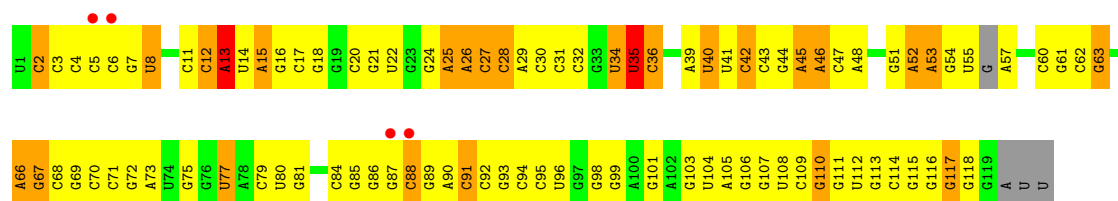
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| C2746 | C2683 | U2555 | A2495 | A2434 | G2373 | C2313 | G2253 | C2183 | G2123 | A2062 | G2002 | U1940 | C1880 |
| U2747 | U2684 | G2556 | G2496 | A2435 | C2374 | C2314 | G2254 | G2184 | G2124 | C2063 | G2003 | C1941 | C1881 |
| G2747 | G2685 | G2557 | A2497 | G2436 | G2375 | G2315 | G2255 | C2185 | G2125 | C2064 | G2004 | C1942 | C1882 |
| A2748 | G2686 | C2558 | C2488 | U2437 | A2376 | C2316 | G2256 | G2186 | A2126 | C2065 | A2005 | U1943 | G1883 |
| U2749 | U2687 | C2559 | G2499 | U2438 | A2377 | C2317 | U2257 | G2187 | G2127 | C2066 | C2006 | U1944 | A1884 |
| A2750 | U2688 | C2560 | U2500 | A2439 | A2378 | G2318 | G2258 | C2188 | G2128 | G2067 | C2007 | G1945 | A1885 |
| G2751 | U2689 | A2561 | G2501 | G2440 | G2379 | G2319 | G2259 | U2189 | C2129 | U2068 | G2008 | U1946 | C1886 |
| C2752 | C2690 | U2562 | G2502 | C2441 | C2381 | G2321 | C2261 | G2190 | U2130 | G2069 | G2009 | C1947 | C1887 |
| A2753 | C2691 | U2563 | A2503 | C2442 | G2382 | G2322 | C2262 | G2191 | G2131 | G2070 | G2010 | G1948 | G1888 |
| U2754 | C2692 | A2564 | U2504 | C2443 | G2383 | A2323 | U2263 | G2192 | U2132 | A2071 | U2011 | A1889 | A1889 |
| C2755 | A2693 | A2565 | G2505 | G2444 | G2384 | G2324 | C2264 | G2193 | G2133 | G2072 | G2012 | U1951 | A1890 |
| U2756 | G2694 | A2566 | U2506 | G2445 | G2385 | G2325 | C2265 | G2194 | A2134 | C2073 | A2013 | A1952 | G1891 |
| A2757 | C2695 | G2567 | G2507 | G2446 | C2386 | G2326 | U2266 | C2195 | U2074 | U2075 | A2014 | A1953 | C1892 |
| U2758 | G2696 | G2568 | G2508 | G2447 | C2387 | G2327 | A2267 | G2196 | U2076 | U2076 | A2015 | G1954 | C1893 |
| G2759 | U2697 | C2569 | U2509 | A2448 | U2387 | A2327 | A2268 | U2197 | G2077 | U2077 | U2016 | U1955 | C1894 |
| G2760 | U2698 | G2570 | C2510 | U2449 | A2388 | A2328 | A2269 | U2198 | C2138 | A2077 | U2017 | U1956 | C1895 |
| G2762 | C2699 | U2571 | U2511 | A2450 | A2389 | G2329 | G2270 | A2199 | C2139 | C2078 | G2018 | U1957 | G1896 |
| C2763 | C2700 | A2572 | A2451 | G2450 | U2390 | G2330 | G2271 | C2200 | A2019 | C2079 | A2019 | C1958 | G1897 |
| A2764 | U2636 | C2573 | C2513 | C2452 | G2391 | G2331 | G2271 | C2201 | G2141 | G2080 | A2020 | G1959 | U1898 |



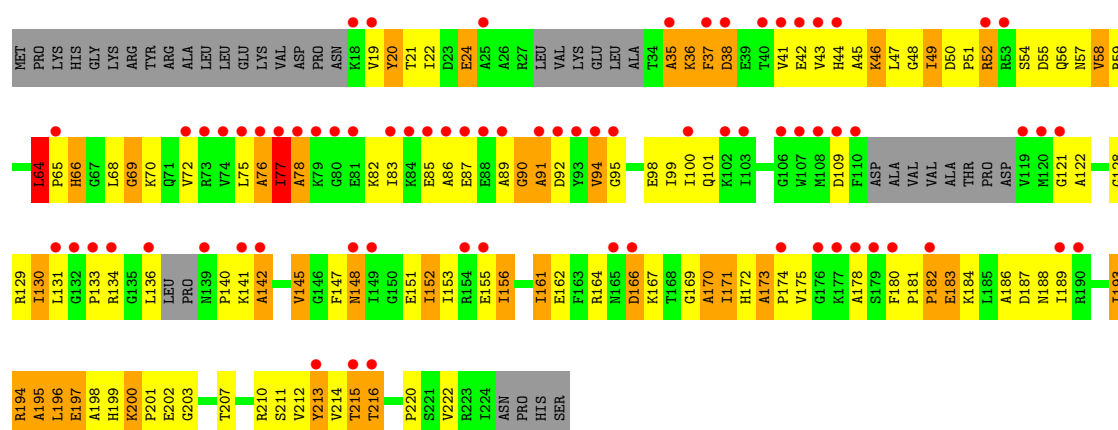
• Molecule 28: 5S ribosomal RNA



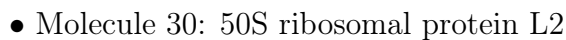
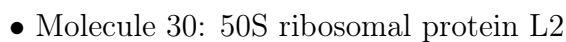
• Molecule 28: 5S ribosomal RNA



• Molecule 29: 50S ribosomal protein L1

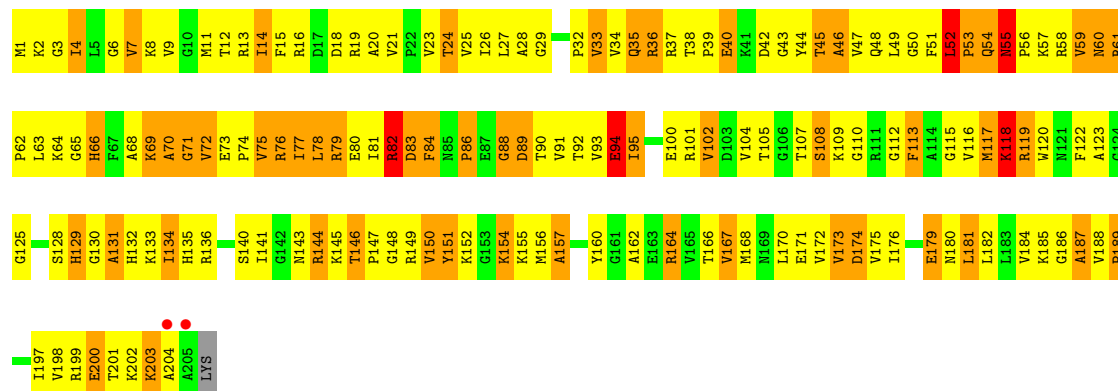


• Molecule 29: 50S ribosomal protein L1

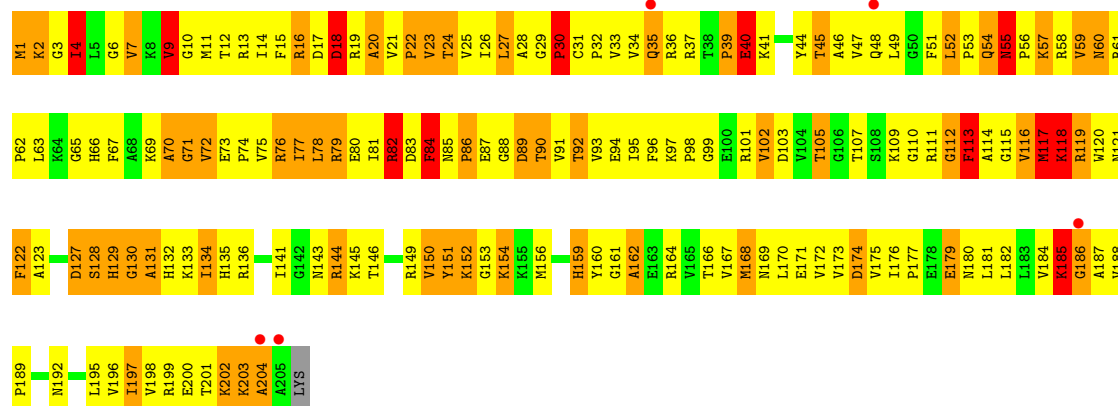




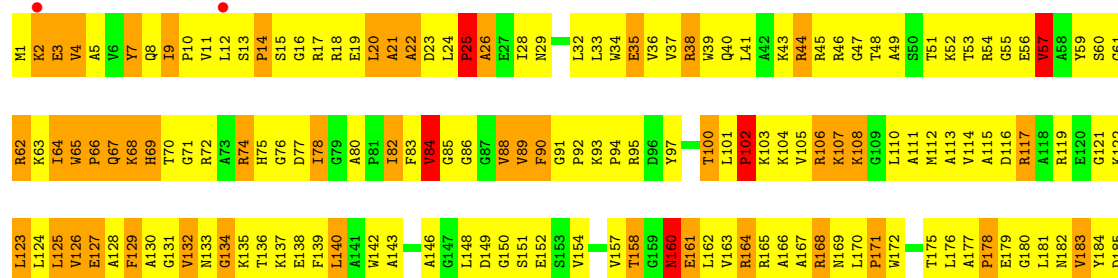
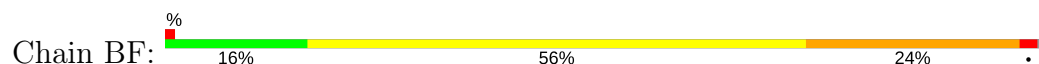
• Molecule 31: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L3

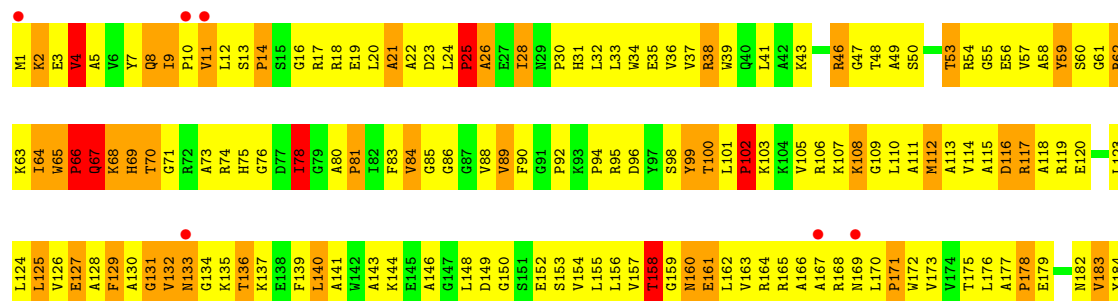
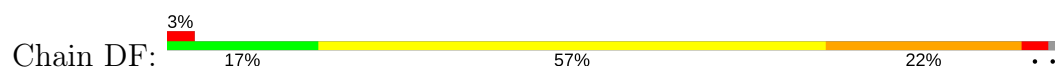


• Molecule 32: 50S ribosomal protein L4

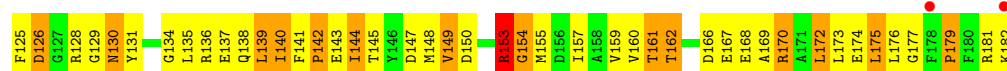
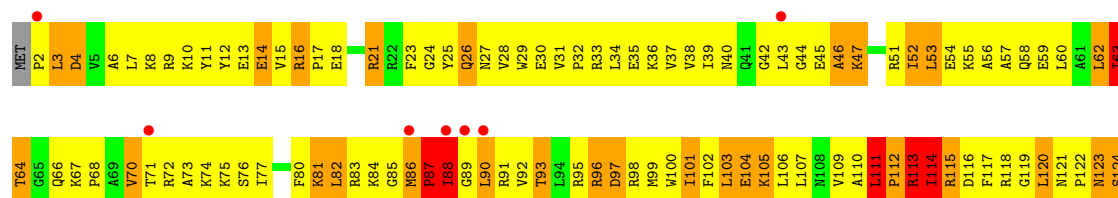
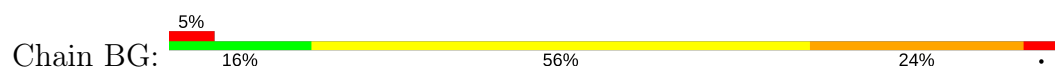




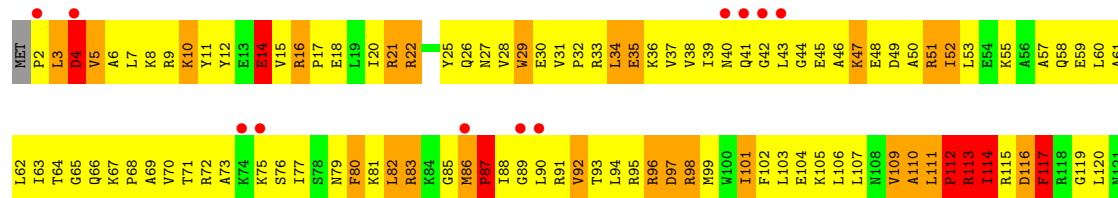
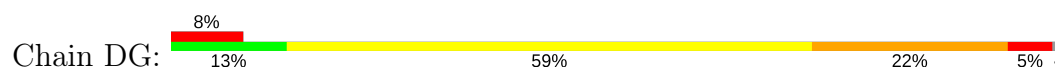
• Molecule 32: 50S ribosomal protein L4



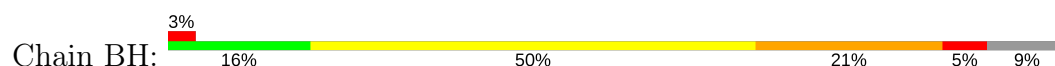
• Molecule 33: 50S ribosomal protein L5



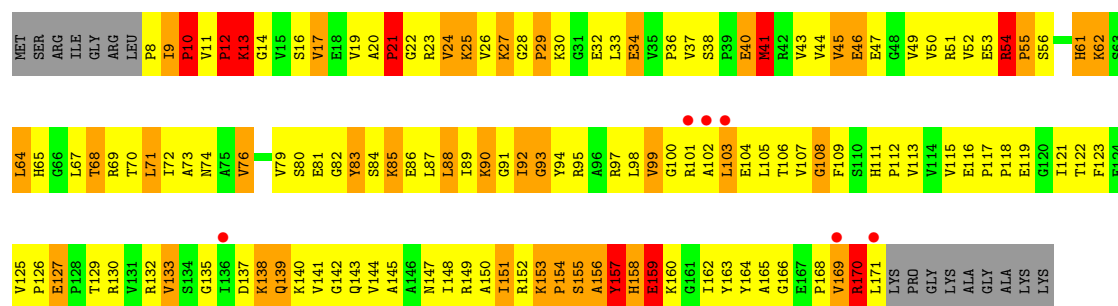
• Molecule 33: 50S ribosomal protein L5



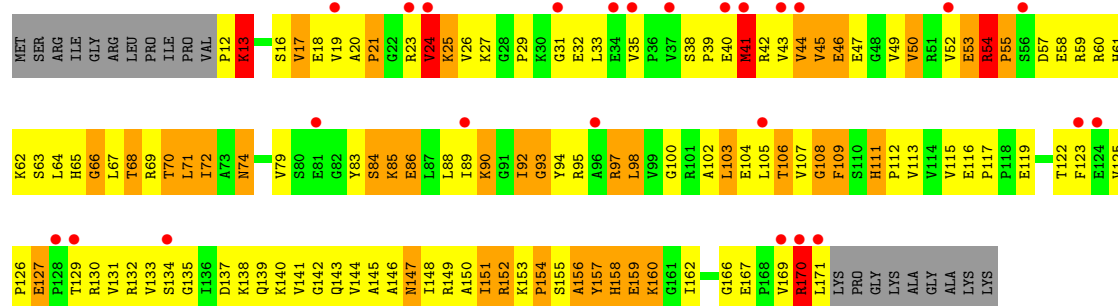
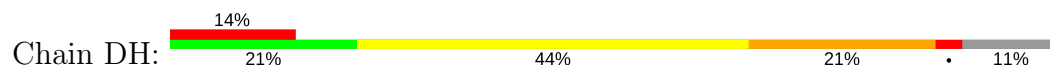
• Molecule 34: 50S ribosomal protein L6



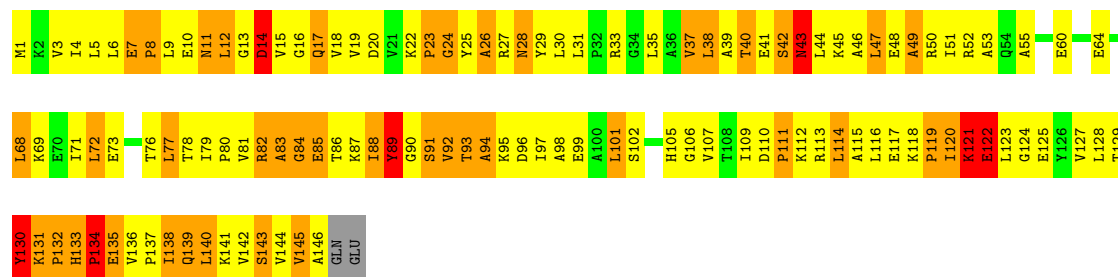
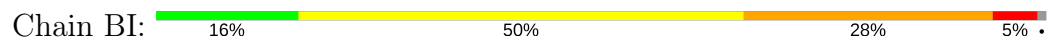




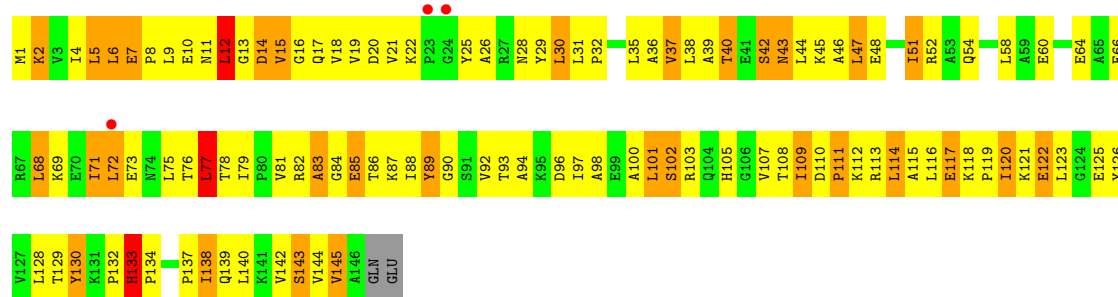
• Molecule 34: 50S ribosomal protein L6



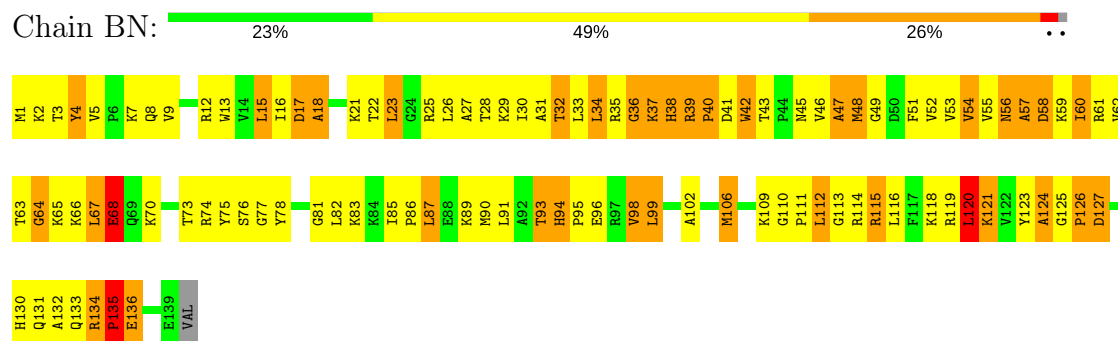
• Molecule 35: 50S ribosomal protein L9



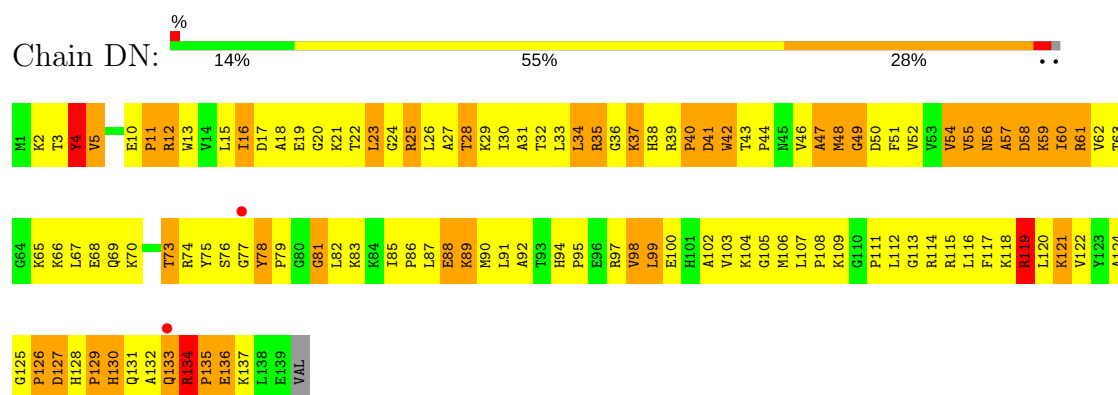
• Molecule 35: 50S ribosomal protein L9



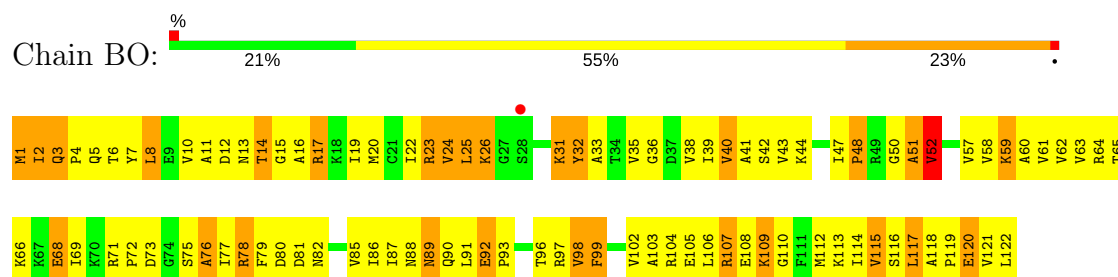
• Molecule 36: 50S ribosomal protein L13



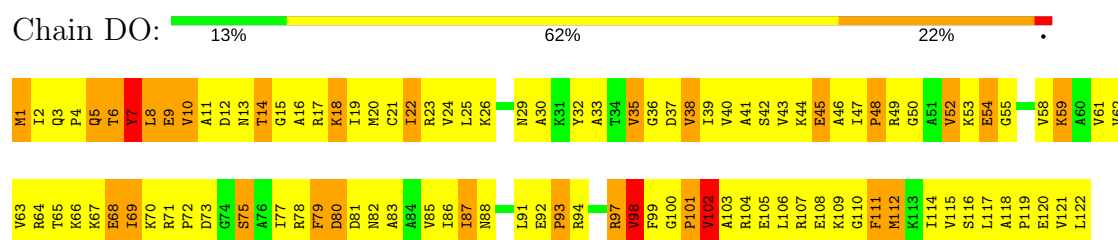
• Molecule 36: 50S ribosomal protein L13



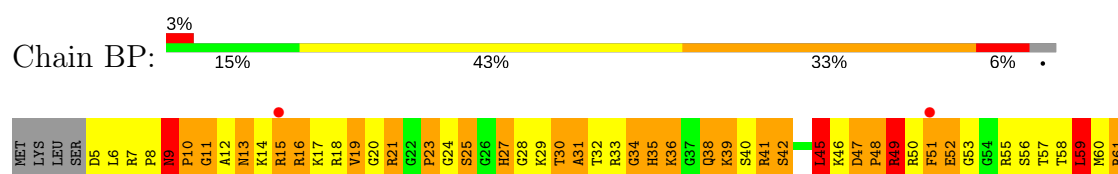
• Molecule 37: 50S ribosomal protein L14

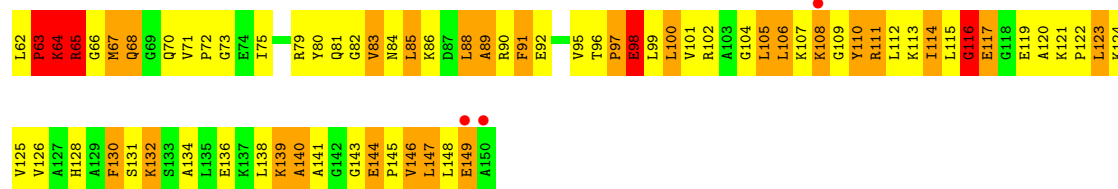


• Molecule 37: 50S ribosomal protein L14

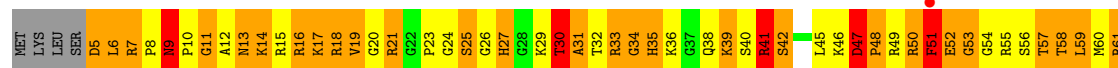


• Molecule 38: 50S ribosomal protein L15





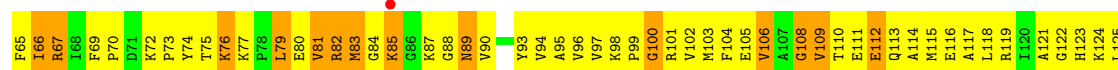
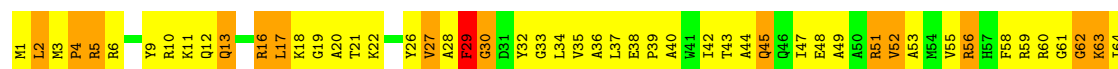
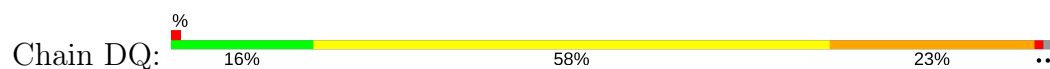
• Molecule 38: 50S ribosomal protein L15



• Molecule 39: 50S ribosomal protein L16

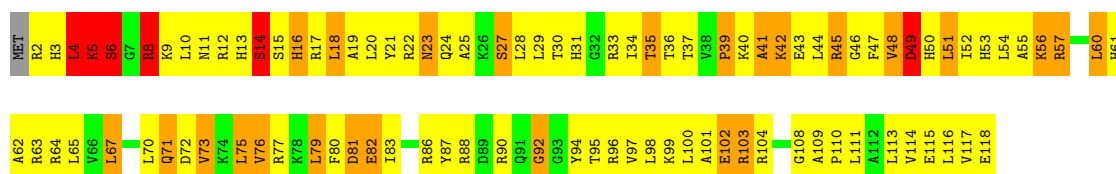


• Molecule 39: 50S ribosomal protein L16



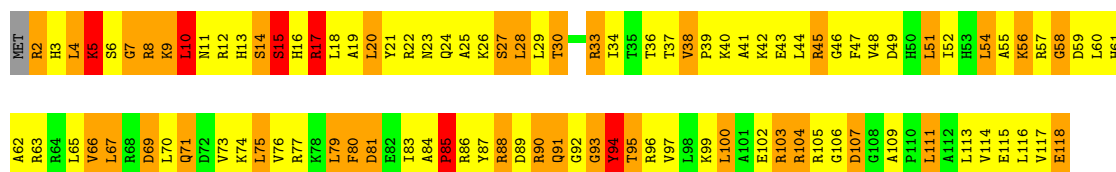
• Molecule 40: 50S ribosomal protein L17





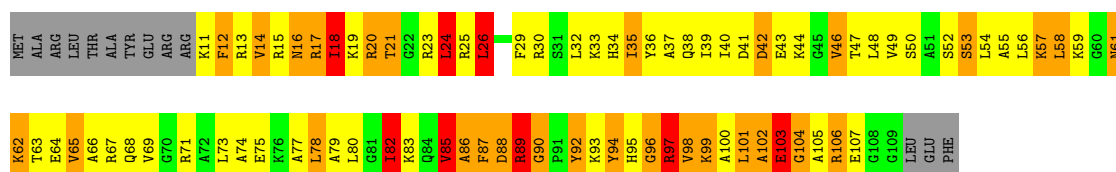
• Molecule 40: 50S ribosomal protein L17

Chain DR: 13% 51% 31% 5%



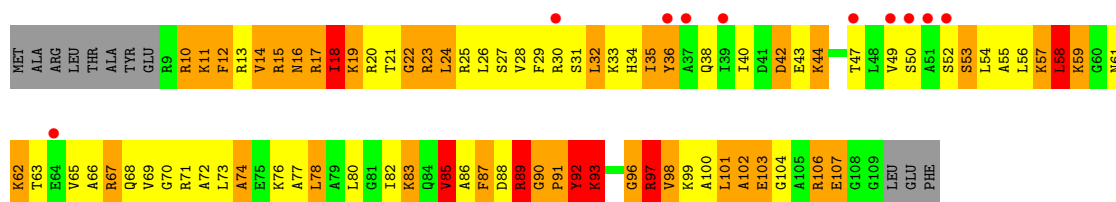
• Molecule 41: 50S ribosomal protein L18

Chain BS: 13% 42% 26% 7% 12%



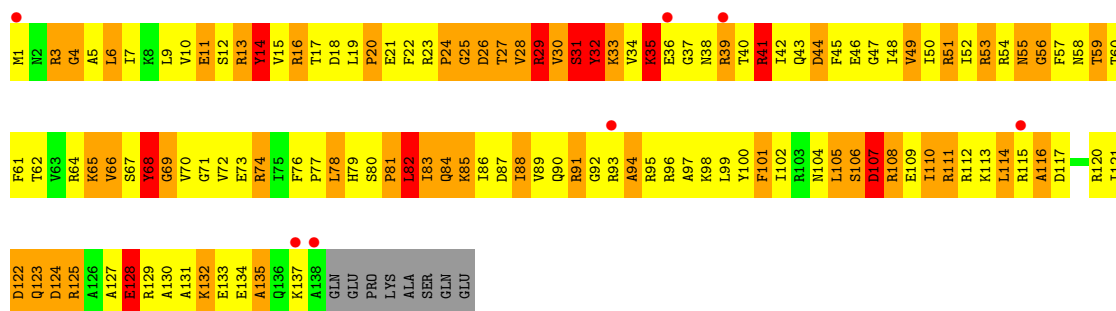
• Molecule 41: 50S ribosomal protein L18

Chain DS: 9% 17% 37% 30% 6% 10%



• Molecule 42: 50S ribosomal protein L19

Chain BT: 5% 7% 48% 33% 7% 5%

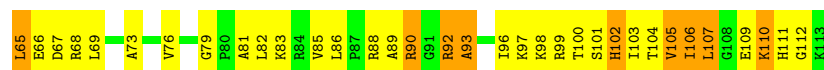
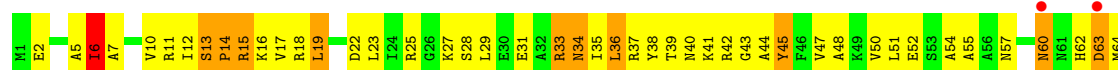


• Molecule 42: 50S ribosomal protein L19

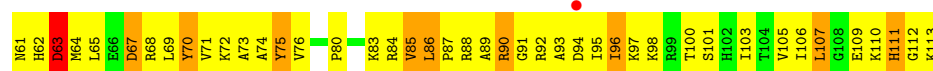




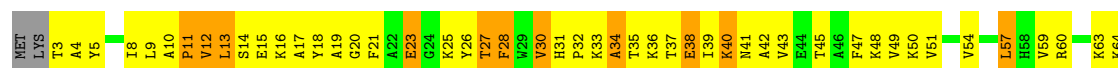
- Molecule 45: 50S ribosomal protein L22



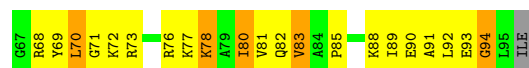
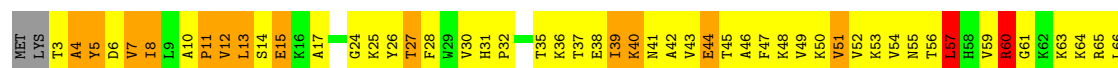
- Molecule 45: 50S ribosomal protein L22



- Molecule 46: 50S ribosomal protein L23



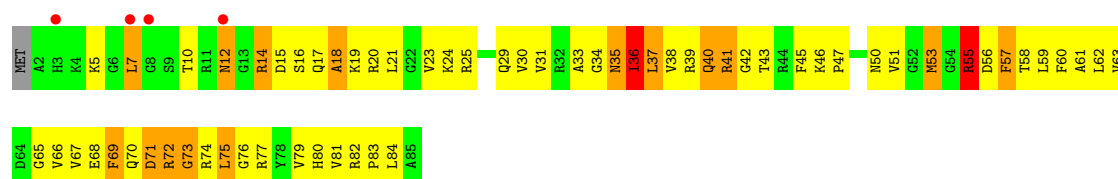
- Molecule 46: 50S ribosomal protein L23



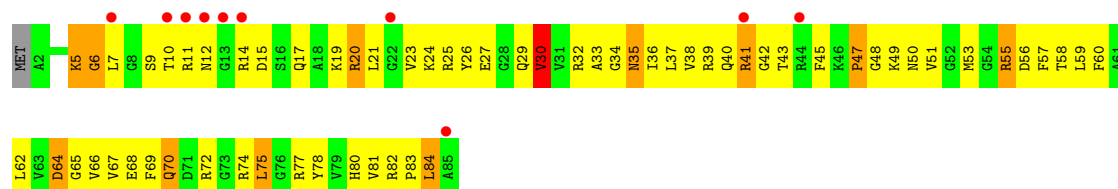
- Molecule 47: 50S ribosomal protein L24



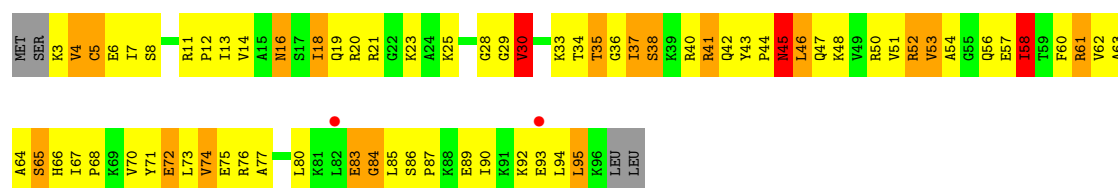




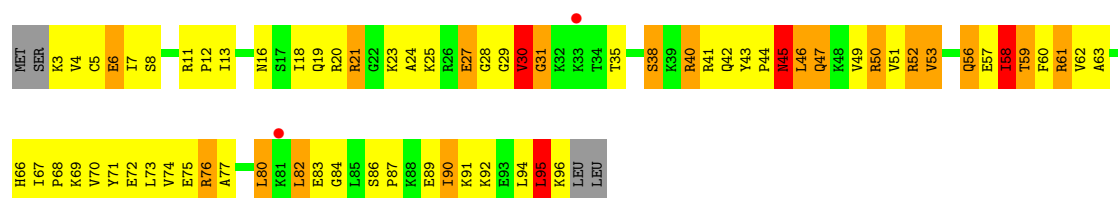
• Molecule 49: 50S ribosomal protein L27



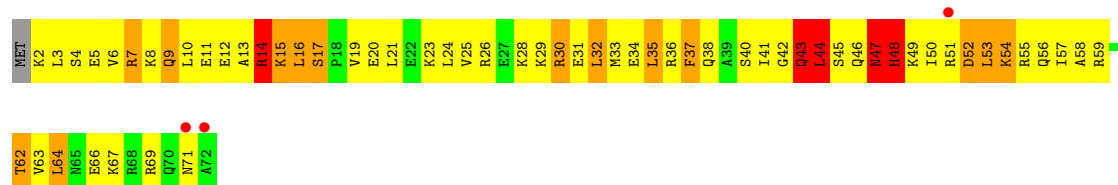
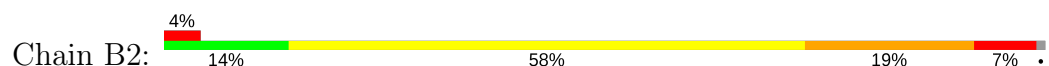
• Molecule 50: 50S ribosomal protein L28



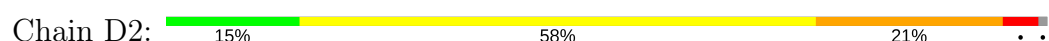
• Molecule 50: 50S ribosomal protein L28



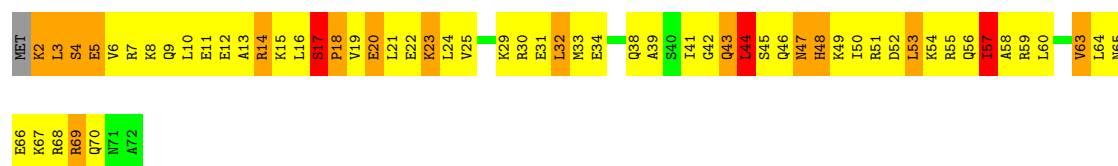
• Molecule 51: 50S ribosomal protein L29



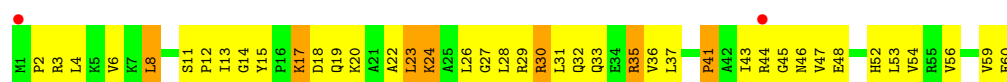
• Molecule 51: 50S ribosomal protein L29



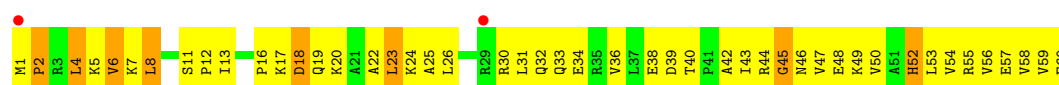




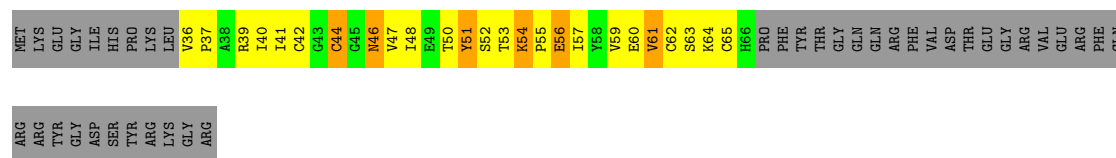
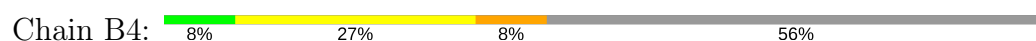
- Molecule 52: 50S ribosomal protein L30



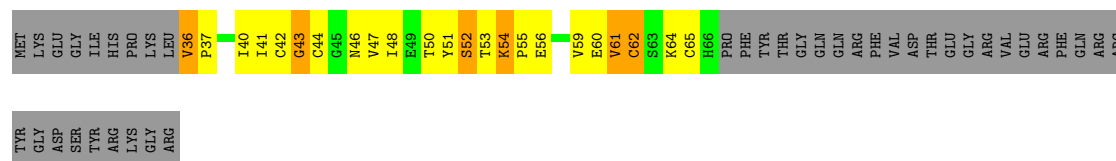
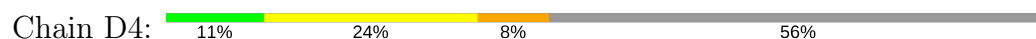
- Molecule 52: 50S ribosomal protein L30



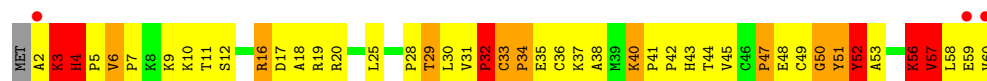
- Molecule 53: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L31



- Molecule 54: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L32





- Molecule 55: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L33



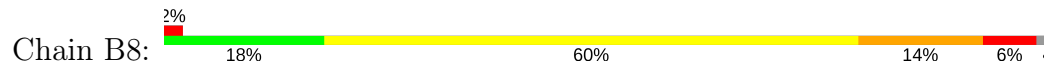
- Molecule 56: 50S ribosomal protein L34



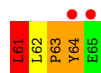
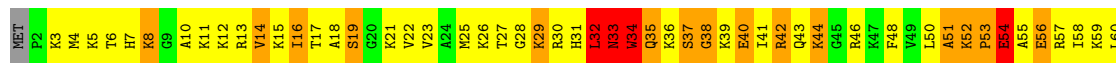
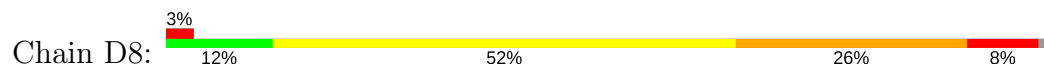
- Molecule 56: 50S ribosomal protein L34



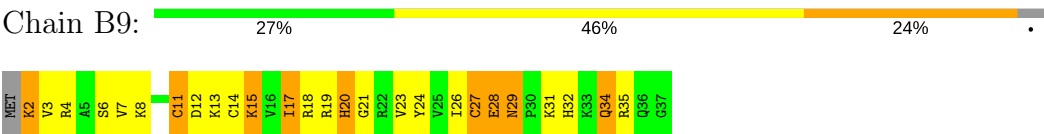
- Molecule 57: 50S ribosomal protein L35



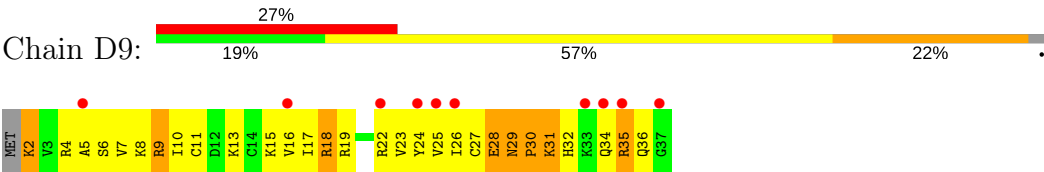
- Molecule 57: 50S ribosomal protein L35



● Molecule 58: 50S ribosomal protein L36



● Molecule 58: 50S ribosomal protein L36



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.23Å 448.51Å 633.62Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 50.00 – 3.00<br>49.93 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (50.00-3.00)<br>94.2 (49.93-3.00)           | Depositor<br>EDS |
| $R_{merge}$   | 0.31  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.01 (at 3.01Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.248 , 0.272<br>0.252 , 0.283                              | Depositor<br>DCC |
| $R_{free}$ test set   | 55515 reflections (5.27%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 88.5  | Xtriage          |
| Anisotropy  | 0.155   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 91.4   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 294559  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 86.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: ZN, DPP, MG, KBE, UAL, 5OH

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    | 0.52         | 0/35980      | 0.82        | 47/56157 (0.1%) |
| 1   | CA    | 0.50         | 0/35980      | 0.82        | 32/56157 (0.1%) |
| 2   | AB    | 0.38         | 0/1936       | 0.73        | 0/2611          |
| 2   | CB    | 0.37         | 0/1936       | 0.71        | 0/2611          |
| 3   | AC    | 0.37         | 0/1637       | 0.74        | 1/2207 (0.0%)   |
| 3   | CC    | 0.37         | 0/1637       | 0.73        | 0/2207          |
| 4   | AD    | 0.45         | 0/1733       | 0.76        | 1/2318 (0.0%)   |
| 4   | CD    | 0.44         | 0/1733       | 0.80        | 2/2318 (0.1%)   |
| 5   | AE    | 0.43         | 0/1163       | 0.77        | 0/1566          |
| 5   | CE    | 0.43         | 0/1163       | 0.77        | 0/1566          |
| 6   | AF    | 0.41         | 0/856        | 0.71        | 0/1154          |
| 6   | CF    | 0.41         | 0/856        | 0.72        | 0/1154          |
| 7   | AG    | 0.39         | 0/1276       | 0.75        | 1/1709 (0.1%)   |
| 7   | CG    | 0.40         | 0/1276       | 0.69        | 0/1709          |
| 8   | AH    | 0.42         | 0/1136       | 0.76        | 0/1527          |
| 8   | CH    | 0.40         | 0/1136       | 0.73        | 0/1527          |
| 9   | AI    | 0.36         | 0/1023       | 0.71        | 0/1371          |
| 9   | CI    | 0.37         | 0/1024       | 0.68        | 0/1372          |
| 10  | AJ    | 0.37         | 0/808        | 0.68        | 0/1087          |
| 10  | CJ    | 0.39         | 0/808        | 0.72        | 0/1087          |
| 11  | AK    | 0.40         | 0/900        | 0.77        | 1/1213 (0.1%)   |
| 11  | CK    | 0.41         | 0/900        | 0.77        | 1/1213 (0.1%)   |
| 12  | AL    | 0.47         | 0/987        | 0.89        | 0/1322          |
| 12  | CL    | 0.43         | 0/987        | 0.79        | 0/1322          |
| 13  | AM    | 0.44         | 0/957        | 0.80        | 0/1284          |
| 13  | CM    | 0.89         | 5/920 (0.5%) | 1.22        | 13/1241 (1.0%)  |
| 14  | AN    | 0.43         | 0/501        | 0.73        | 0/664           |
| 14  | CN    | 0.42         | 0/501        | 0.72        | 1/664 (0.2%)    |
| 15  | AO    | 0.43         | 0/745        | 0.71        | 0/992           |
| 15  | CO    | 0.41         | 0/745        | 0.67        | 0/992           |
| 16  | AP    | 0.43         | 0/717        | 0.78        | 1/965 (0.1%)    |
| 16  | CP    | 0.40         | 0/717        | 0.70        | 0/965           |

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5          |
| 17  | AQ    | 0.44         | 0/837         | 0.77        | 0/1119           |
| 17  | CQ    | 0.40         | 0/837         | 0.74        | 0/1119           |
| 18  | AR    | 0.45         | 0/579         | 0.82        | 0/768            |
| 18  | CR    | 0.44         | 0/579         | 0.82        | 0/768            |
| 19  | AS    | 0.41         | 0/643         | 0.71        | 0/867            |
| 19  | CS    | 0.39         | 0/643         | 0.69        | 0/867            |
| 20  | AT    | 0.38         | 0/765         | 0.80        | 0/1007           |
| 20  | CT    | 0.39         | 0/765         | 0.77        | 0/1007           |
| 21  | AU    | 0.46         | 0/213         | 0.77        | 0/279            |
| 21  | CU    | 0.36         | 0/213         | 0.66        | 0/279            |
| 22  | AV    | 0.56         | 0/239         | 0.66        | 0/371            |
| 22  | CV    | 0.49         | 0/239         | 0.81        | 1/371 (0.3%)     |
| 23  | AW    | 0.50         | 0/1778        | 0.76        | 0/2768           |
| 23  | CW    | 0.43         | 0/1778        | 0.74        | 0/2768           |
| 24  | AX    | 0.50         | 0/1832        | 0.74        | 0/2855           |
| 24  | CX    | 0.49         | 0/1832        | 0.73        | 1/2855 (0.0%)    |
| 25  | AY    | 0.36         | 0/1776        | 0.71        | 0/2766           |
| 25  | CY    | 0.39         | 0/1776        | 0.73        | 0/2766           |
| 26  | AZ    | 0.95         | 0/11          | 0.62        | 0/13             |
| 26  | CZ    | 1.05         | 0/11          | 0.87        | 0/13             |
| 27  | BA    | 0.64         | 0/67544       | 0.87        | 94/105433 (0.1%) |
| 27  | DA    | 0.55         | 0/67547       | 0.85        | 93/105438 (0.1%) |
| 28  | BB    | 0.58         | 0/2826        | 0.85        | 4/4406 (0.1%)    |
| 28  | DB    | 0.50         | 0/2826        | 0.85        | 4/4406 (0.1%)    |
| 29  | BC    | 0.29         | 0/1145        | 0.64        | 0/1556           |
| 29  | DC    | 0.30         | 0/1145        | 0.67        | 0/1556           |
| 30  | BD    | 0.60         | 2/2155 (0.1%) | 0.94        | 3/2907 (0.1%)    |
| 30  | DD    | 0.52         | 0/2155        | 0.90        | 5/2907 (0.2%)    |
| 31  | BE    | 0.55         | 0/1597        | 0.92        | 0/2155           |
| 31  | DE    | 0.46         | 0/1597        | 0.89        | 3/2155 (0.1%)    |
| 32  | BF    | 0.50         | 0/1659        | 0.83        | 0/2246           |
| 32  | DF    | 0.44         | 0/1659        | 0.81        | 1/2246 (0.0%)    |
| 33  | BG    | 0.52         | 1/1499 (0.1%) | 0.91        | 5/2016 (0.2%)    |
| 33  | DG    | 0.50         | 1/1499 (0.1%) | 0.89        | 5/2016 (0.2%)    |
| 34  | BH    | 0.54         | 1/1277 (0.1%) | 0.89        | 3/1729 (0.2%)    |
| 34  | DH    | 0.35         | 0/1246        | 0.76        | 0/1684           |
| 35  | BI    | 0.37         | 0/1057        | 0.81        | 0/1453           |
| 35  | DI    | 0.38         | 0/1061        | 0.81        | 0/1458           |
| 36  | BN    | 0.54         | 0/1132        | 0.89        | 2/1527 (0.1%)    |
| 36  | DN    | 0.41         | 0/1132        | 0.79        | 0/1527           |
| 37  | BO    | 0.50         | 0/943         | 0.90        | 4/1269 (0.3%)    |
| 37  | DO    | 0.48         | 0/943         | 0.79        | 0/1269           |
| 38  | BP    | 0.60         | 0/1131        | 1.14        | 9/1504 (0.6%)    |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 38  | DP    | 0.49         | 0/1131           | 0.97        | 5/1504 (0.3%)     |
| 39  | BQ    | 0.52         | 0/1143           | 0.79        | 0/1527            |
| 39  | DQ    | 0.41         | 0/1128           | 0.73        | 0/1508            |
| 40  | BR    | 0.53         | 0/974            | 0.94        | 6/1302 (0.5%)     |
| 40  | DR    | 0.45         | 0/974            | 0.87        | 2/1302 (0.2%)     |
| 41  | BS    | 0.50         | 0/779            | 1.01        | 4/1038 (0.4%)     |
| 41  | DS    | 0.42         | 0/785            | 0.92        | 3/1048 (0.3%)     |
| 42  | BT    | 0.54         | 0/1156           | 0.99        | 5/1544 (0.3%)     |
| 42  | DT    | 0.48         | 0/1156           | 0.89        | 2/1544 (0.1%)     |
| 43  | BU    | 0.57         | 0/975            | 0.86        | 2/1297 (0.2%)     |
| 43  | DU    | 0.42         | 0/975            | 0.84        | 3/1297 (0.2%)     |
| 44  | BV    | 0.51         | 0/790            | 0.95        | 3/1057 (0.3%)     |
| 44  | DV    | 0.42         | 0/790            | 0.82        | 0/1057            |
| 45  | BW    | 0.52         | 0/907            | 0.88        | 2/1216 (0.2%)     |
| 45  | DW    | 0.50         | 0/907            | 0.85        | 0/1216            |
| 46  | BX    | 0.53         | 0/740            | 0.89        | 0/995             |
| 46  | DX    | 0.48         | 0/740            | 0.81        | 1/995 (0.1%)      |
| 47  | BY    | 0.56         | 0/789            | 1.06        | 3/1053 (0.3%)     |
| 47  | DY    | 0.48         | 0/789            | 0.93        | 3/1053 (0.3%)     |
| 48  | BZ    | 0.42         | 0/1436           | 0.74        | 0/1951            |
| 48  | DZ    | 0.36         | 0/1436           | 0.70        | 0/1951            |
| 49  | B0    | 0.53         | 0/671            | 0.81        | 1/892 (0.1%)      |
| 49  | D0    | 0.45         | 0/671            | 0.73        | 0/892             |
| 50  | B1    | 0.49         | 0/722            | 0.82        | 0/964             |
| 50  | D1    | 0.47         | 0/739            | 0.79        | 0/983             |
| 51  | B2    | 0.55         | 0/600            | 0.86        | 1/793 (0.1%)      |
| 51  | D2    | 0.42         | 0/600            | 0.74        | 0/793             |
| 52  | B3    | 0.52         | 0/473            | 0.84        | 0/636             |
| 52  | D3    | 0.41         | 0/473            | 0.81        | 0/636             |
| 53  | B4    | 0.42         | 0/229            | 0.86        | 0/311             |
| 53  | D4    | 0.50         | 0/229            | 1.01        | 2/311 (0.6%)      |
| 54  | B5    | 0.53         | 0/473            | 0.95        | 2/639 (0.3%)      |
| 54  | D5    | 0.46         | 0/473            | 0.79        | 0/639             |
| 55  | B6    | 0.75         | 0/418            | 1.17        | 3/562 (0.5%)      |
| 55  | D6    | 0.80         | 1/397 (0.3%)     | 1.20        | 4/531 (0.8%)      |
| 56  | B7    | 0.59         | 0/427            | 0.92        | 1/563 (0.2%)      |
| 56  | D7    | 0.50         | 0/427            | 0.85        | 0/563             |
| 57  | B8    | 0.59         | 0/516            | 1.01        | 1/681 (0.1%)      |
| 57  | D8    | 0.50         | 0/516            | 0.95        | 3/681 (0.4%)      |
| 58  | B9    | 0.54         | 0/302            | 0.88        | 0/397             |
| 58  | D9    | 0.33         | 0/302            | 0.74        | 0/397             |
| All | All   | 0.54         | 11/318953 (0.0%) | 0.84        | 400/477060 (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 |
|-----|-------|---------------------|---------------------|
| 1   | AA    | 0                   | 90                  |
| 1   | CA    | 1                   | 81                  |
| 13  | CM    | 0                   | 1                   |
| 22  | CV    | 0                   | 2                   |
| 23  | AW    | 0                   | 1                   |
| 23  | CW    | 0                   | 2                   |
| 27  | BA    | 0                   | 223                 |
| 27  | DA    | 0                   | 164                 |
| 28  | BB    | 0                   | 6                   |
| 28  | DB    | 0                   | 6                   |
| 30  | DD    | 0                   | 1                   |
| 36  | DN    | 0                   | 1                   |
| 47  | BY    | 0                   | 1                   |
| 54  | D5    | 0                   | 1                   |
| 55  | B6    | 0                   | 1                   |
| 55  | D6    | 0                   | 1                   |
| All | All   | 1                   | 582                 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 13  | CM    | 113 | PRO  | N-CD  | -7.63 | 1.37        | 1.47     |
| 55  | D6    | 46  | HIS  | C-N   | -6.65 | 1.18        | 1.34     |
| 34  | BH    | 11  | VAL  | C-N   | 6.53  | 1.46        | 1.34     |
| 13  | CM    | 65  | LYS  | C-N   | 6.24  | 1.48        | 1.34     |
| 33  | BG    | 111 | LEU  | C-N   | 5.78  | 1.45        | 1.34     |
| 30  | BD    | 246 | PRO  | N-CD  | 5.75  | 1.55        | 1.47     |
| 13  | CM    | 112 | GLY  | C-O   | -5.56 | 1.14        | 1.23     |
| 13  | CM    | 65  | LYS  | CA-C  | 5.43  | 1.67        | 1.52     |
| 13  | CM    | 72  | ALA  | CA-CB | 5.31  | 1.63        | 1.52     |
| 30  | BD    | 245 | PRO  | C-N   | -5.22 | 1.24        | 1.34     |
| 33  | DG    | 111 | LEU  | C-N   | 5.21  | 1.44        | 1.34     |

All (400) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 13  | CM    | 70   | LEU  | N-CA-C     | -12.04 | 78.50       | 111.00   |
| 27  | BA    | 2424 | C    | N1-C1'-C2' | -11.64 | 98.86       | 114.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 55  | B6    | 46   | HIS  | N-CA-C      | 11.54  | 142.16      | 111.00   |
| 38  | BP    | 52   | GLU  | N-CA-C      | 11.01  | 140.73      | 111.00   |
| 27  | DA    | 1782 | C    | N1-C1'-C2'  | -10.49 | 100.36      | 114.00   |
| 55  | D6    | 46   | HIS  | N-CA-C      | 10.23  | 138.63      | 111.00   |
| 1   | AA    | 52   | G    | N9-C1'-C2'  | -10.22 | 100.71      | 114.00   |
| 27  | DA    | 1992 | G    | N9-C1'-C2'  | 10.09  | 127.12      | 114.00   |
| 38  | BP    | 116  | GLY  | N-CA-C      | 9.33   | 136.42      | 113.10   |
| 1   | CA    | 517  | G    | C2'-C3'-O3' | 9.26   | 129.88      | 109.50   |
| 38  | DP    | 52   | GLU  | N-CA-C      | 9.24   | 135.96      | 111.00   |
| 1   | CA    | 874  | G    | N9-C1'-C2'  | -8.89  | 102.22      | 112.00   |
| 27  | DA    | 226  | G    | C2'-C3'-O3' | 8.89   | 129.06      | 109.50   |
| 1   | AA    | 508  | C    | C2'-C3'-O3' | 8.64   | 128.51      | 109.50   |
| 13  | CM    | 70   | LEU  | CB-CG-CD1   | -8.56  | 96.44       | 111.00   |
| 13  | CM    | 70   | LEU  | CB-CG-CD2   | -8.41  | 96.71       | 111.00   |
| 1   | AA    | 131  | C    | N1-C1'-C2'  | -8.40  | 102.76      | 112.00   |
| 13  | CM    | 69   | GLU  | O-C-N       | 8.30   | 135.98      | 122.70   |
| 1   | CA    | 199  | G    | N9-C1'-C2'  | -8.20  | 102.98      | 112.00   |
| 1   | CA    | 533  | A    | C2'-C3'-O3' | 8.13   | 127.38      | 109.50   |
| 27  | BA    | 1992 | G    | C2'-C3'-O3' | 8.11   | 127.34      | 109.50   |
| 47  | DY    | 54   | LYS  | N-CA-C      | -7.86  | 89.79       | 111.00   |
| 1   | AA    | 266  | G    | C2'-C3'-O3' | 7.78   | 126.61      | 109.50   |
| 27  | BA    | 467  | G    | N9-C1'-C2'  | -7.76  | 103.46      | 112.00   |
| 27  | DA    | 421  | U    | C2'-C3'-O3' | 7.74   | 126.52      | 109.50   |
| 27  | DA    | 2873 | A    | C5'-C4'-O4' | 7.72   | 118.37      | 109.10   |
| 1   | AA    | 498  | U    | N1-C1'-C2'  | -7.63  | 103.61      | 112.00   |
| 1   | AA    | 1265 | G    | N9-C1'-C2'  | -7.55  | 103.69      | 112.00   |
| 27  | BA    | 329  | G    | C2'-C3'-O3' | 7.54   | 126.08      | 109.50   |
| 38  | BP    | 53   | GLY  | N-CA-C      | -7.54  | 94.26       | 113.10   |
| 27  | DA    | 1289 | C    | N1-C1'-C2'  | -7.44  | 103.81      | 112.00   |
| 30  | BD    | 245  | PRO  | N-CA-C      | -7.44  | 92.76       | 112.10   |
| 13  | CM    | 65   | LYS  | CA-CB-CG    | -7.40  | 97.11       | 113.40   |
| 27  | BA    | 2776 | A    | C2'-C3'-O3' | 7.37   | 125.72      | 109.50   |
| 27  | DA    | 1386 | C    | N1-C1'-C2'  | -7.36  | 103.91      | 112.00   |
| 27  | BA    | 996  | A    | N9-C1'-C2'  | -7.34  | 103.92      | 112.00   |
| 1   | AA    | 1077 | G    | N9-C1'-C2'  | -7.31  | 103.96      | 112.00   |
| 27  | DA    | 2525 | G    | N9-C1'-C2'  | -7.30  | 103.97      | 112.00   |
| 27  | BA    | 1126 | A    | C2'-C3'-O3' | 7.29   | 125.54      | 109.50   |
| 33  | DG    | 114  | ILE  | N-CA-C      | -7.26  | 91.41       | 111.00   |
| 38  | DP    | 53   | GLY  | N-CA-C      | -7.23  | 95.02       | 113.10   |
| 27  | DA    | 2127 | G    | N9-C1'-C2'  | -7.20  | 104.08      | 112.00   |
| 43  | DU    | 78   | THR  | N-CA-C      | -7.15  | 91.69       | 111.00   |
| 1   | AA    | 140  | A    | N9-C1'-C2'  | -7.12  | 104.17      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31  | DE    | 186  | GLY  | N-CA-C      | 7.11  | 130.88      | 113.10   |
| 41  | DS    | 16   | ASN  | N-CA-C      | -7.09 | 91.86       | 111.00   |
| 31  | DE    | 87   | GLU  | N-CA-C      | -7.07 | 91.90       | 111.00   |
| 1   | AA    | 578  | C    | N1-C1'-C2'  | -7.06 | 104.24      | 112.00   |
| 27  | DA    | 1781 | C    | O4'-C1'-N1  | 7.05  | 113.84      | 108.20   |
| 1   | AA    | 1067 | A    | C2'-C3'-O3' | 7.04  | 124.98      | 109.50   |
| 36  | BN    | 18   | ALA  | N-CA-C      | -7.03 | 92.02       | 111.00   |
| 1   | AA    | 494  | U    | N1-C1'-C2'  | -7.02 | 104.28      | 112.00   |
| 33  | DG    | 112  | PRO  | N-CA-CB     | -7.01 | 94.89       | 102.60   |
| 1   | AA    | 1196 | U    | N1-C1'-C2'  | 7.01  | 123.11      | 114.00   |
| 27  | DA    | 831  | G    | C5'-C4'-C3' | -6.95 | 104.88      | 116.00   |
| 55  | D6    | 48   | VAL  | N-CA-C      | 6.92  | 129.70      | 111.00   |
| 27  | DA    | 2134 | A    | N9-C1'-C2'  | -6.92 | 104.39      | 112.00   |
| 1   | CA    | 266  | G    | C2'-C3'-O3' | 6.87  | 124.69      | 113.70   |
| 27  | BA    | 2346 | A    | N9-C1'-C2'  | 6.86  | 122.92      | 114.00   |
| 1   | CA    | 1154 | G    | N9-C1'-C2'  | -6.84 | 104.48      | 112.00   |
| 27  | DA    | 1700 | A    | N9-C1'-C2'  | -6.82 | 104.50      | 112.00   |
| 27  | BA    | 2832 | U    | C2'-C3'-O3' | 6.80  | 124.58      | 113.70   |
| 54  | B5    | 52   | TYR  | N-CA-C      | -6.78 | 92.70       | 111.00   |
| 13  | CM    | 64   | TRP  | C-N-CA      | -6.77 | 104.77      | 121.70   |
| 27  | DA    | 467  | G    | N9-C1'-C2'  | -6.76 | 104.57      | 112.00   |
| 38  | BP    | 51   | PHE  | N-CA-C      | 6.75  | 129.23      | 111.00   |
| 27  | BA    | 2491 | U    | O4'-C1'-N1  | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 1021 | G    | N9-C1'-C2'  | -6.74 | 104.59      | 112.00   |
| 30  | DD    | 244  | ARG  | C-N-CD      | -6.73 | 105.79      | 120.60   |
| 47  | DY    | 7    | VAL  | N-CA-C      | 6.71  | 129.13      | 111.00   |
| 1   | AA    | 1461 | G    | N9-C1'-C2'  | -6.71 | 104.62      | 112.00   |
| 28  | DB    | 117  | G    | N9-C1'-C2'  | -6.70 | 104.63      | 112.00   |
| 27  | BA    | 1616 | A    | N9-C1'-C2'  | 6.68  | 122.69      | 114.00   |
| 40  | BR    | 8    | ARG  | N-CA-C      | 6.68  | 129.04      | 111.00   |
| 27  | BA    | 301  | G    | C2'-C3'-O3' | 6.68  | 124.38      | 113.70   |
| 27  | BA    | 2068 | U    | N1-C1'-C2'  | -6.65 | 104.68      | 112.00   |
| 27  | BA    | 2477 | C    | N1-C1'-C2'  | 6.63  | 122.62      | 114.00   |
| 27  | DA    | 548  | A    | O4'-C1'-N9  | 6.59  | 113.47      | 108.20   |
| 27  | DA    | 1786 | A    | N9-C1'-C2'  | 6.59  | 122.57      | 114.00   |
| 33  | BG    | 114  | ILE  | N-CA-C      | -6.56 | 93.30       | 111.00   |
| 27  | DA    | 1945 | G    | N9-C1'-C2'  | -6.56 | 104.79      | 112.00   |
| 27  | BA    | 2820 | A    | C2'-C3'-O3' | 6.55  | 124.19      | 113.70   |
| 30  | BD    | 246  | PRO  | CA-N-CD     | -6.55 | 102.33      | 111.50   |
| 27  | BA    | 2318 | G    | C2'-C3'-O3' | 6.55  | 124.17      | 113.70   |
| 27  | DA    | 1992 | G    | C2'-C3'-O3' | 6.53  | 124.15      | 113.70   |
| 27  | BA    | 2830 | G    | C5'-C4'-C3' | -6.53 | 105.56      | 116.00   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 27  | BA    | 1996   | C    | N1-C1'-C2'  | 6.53  | 122.48      | 114.00   |
| 40  | DR    | 10     | LEU  | CA-CB-CG    | 6.49  | 130.24      | 115.30   |
| 53  | D4    | 62     | CYS  | CA-CB-SG    | -6.49 | 102.32      | 114.00   |
| 34  | BH    | 157    | TYR  | N-CA-C      | -6.49 | 93.49       | 111.00   |
| 13  | CM    | 66     | LEU  | CB-CG-CD2   | -6.49 | 99.97       | 111.00   |
| 27  | BA    | 1947   | C    | C5'-C4'-C3' | -6.47 | 105.65      | 116.00   |
| 27  | BA    | 2036   | C    | N1-C1'-C2'  | -6.46 | 104.90      | 112.00   |
| 27  | BA    | 588    | U    | O5'-P-OP2   | -6.41 | 99.93       | 105.70   |
| 27  | DA    | 33     | U    | C5'-C4'-O4' | 6.39  | 116.76      | 109.10   |
| 57  | B8    | 45     | GLY  | N-CA-C      | -6.38 | 97.15       | 113.10   |
| 30  | DD    | 41     | GLY  | N-CA-C      | -6.36 | 97.19       | 113.10   |
| 27  | BA    | 1698   | A    | N9-C1'-C2'  | 6.36  | 122.27      | 114.00   |
| 27  | DA    | 334    | C    | N1-C1'-C2'  | -6.35 | 105.01      | 112.00   |
| 38  | BP    | 45     | LEU  | N-CA-C      | -6.35 | 93.86       | 111.00   |
| 27  | DA    | 424    | G    | N9-C1'-C2'  | -6.35 | 105.02      | 112.00   |
| 41  | DS    | 18     | ILE  | N-CA-C      | -6.33 | 93.90       | 111.00   |
| 1   | AA    | 792    | A    | C2'-C3'-O3' | 6.33  | 123.83      | 113.70   |
| 27  | DA    | 1653   | G    | C2'-C3'-O3' | 6.33  | 123.83      | 113.70   |
| 49  | B0    | 36     | ILE  | N-CA-C      | -6.28 | 94.06       | 111.00   |
| 1   | AA    | 682    | G    | N9-C1'-C2'  | -6.27 | 105.10      | 112.00   |
| 1   | AA    | 6      | G    | N9-C1'-C2'  | 6.27  | 122.15      | 114.00   |
| 27  | BA    | 729    | G    | N9-C1'-C2'  | 6.22  | 122.09      | 114.00   |
| 1   | CA    | 288    | A    | N9-C1'-C2'  | -6.21 | 105.17      | 112.00   |
| 27  | BA    | 2669   | G    | N9-C1'-C2'  | -6.21 | 105.17      | 112.00   |
| 27  | BA    | 2468   | G    | N9-C1'-C2'  | 6.18  | 122.03      | 114.00   |
| 27  | DA    | 2497   | A    | C2'-C3'-O3' | 6.17  | 123.57      | 113.70   |
| 28  | BB    | 118    | G    | N9-C1'-C2'  | -6.15 | 105.23      | 112.00   |
| 1   | AA    | 785    | G    | C5'-C4'-C3' | -6.15 | 106.16      | 116.00   |
| 1   | CA    | 966    | G    | N9-C1'-C2'  | -6.14 | 105.25      | 112.00   |
| 27  | BA    | 61     | G    | N9-C1'-C2'  | -6.13 | 105.26      | 112.00   |
| 27  | BA    | 1266   | G    | N9-C1'-C2'  | 6.12  | 121.96      | 114.00   |
| 38  | DP    | 51     | PHE  | N-CA-C      | 6.12  | 127.52      | 111.00   |
| 1   | AA    | 189(E) | U    | N1-C1'-C2'  | 6.11  | 121.94      | 114.00   |
| 27  | BA    | 1427   | A    | C2'-C3'-O3' | 6.10  | 123.46      | 113.70   |
| 24  | CX    | 7      | G    | N9-C1'-C2'  | 6.10  | 121.93      | 114.00   |
| 27  | DA    | 1283   | G    | N9-C1'-C2'  | -6.08 | 105.31      | 112.00   |
| 33  | DG    | 129    | GLY  | N-CA-C      | -6.07 | 97.93       | 113.10   |
| 42  | BT    | 29     | ARG  | N-CA-C      | 6.07  | 127.38      | 111.00   |
| 27  | BA    | 1616   | A    | O4'-C1'-N9  | 6.06  | 113.05      | 108.20   |
| 27  | DA    | 1781   | C    | N1-C1'-C2'  | 6.06  | 121.88      | 114.00   |
| 27  | BA    | 856    | C    | C2'-C3'-O3' | 6.05  | 123.38      | 113.70   |
| 1   | AA    | 700    | G    | N9-C1'-C2'  | -6.05 | 105.35      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53  | D4    | 43   | GLY  | N-CA-C      | -6.05 | 97.98       | 113.10   |
| 41  | BS    | 17   | ARG  | N-CA-C      | -6.04 | 94.70       | 111.00   |
| 27  | BA    | 2473 | U    | N1-C1'-C2'  | 6.02  | 121.83      | 114.00   |
| 27  | DA    | 352  | G    | N9-C1'-C2'  | 6.00  | 121.80      | 114.00   |
| 27  | DA    | 1159 | U    | C5'-C4'-C3' | -6.00 | 106.40      | 116.00   |
| 27  | BA    | 44   | G    | N9-C1'-C2'  | -5.98 | 105.43      | 112.00   |
| 27  | DA    | 945  | A    | C5'-C4'-O4' | 5.96  | 116.25      | 109.10   |
| 27  | BA    | 945  | A    | C5'-C4'-O4' | 5.95  | 116.24      | 109.10   |
| 1   | AA    | 331  | G    | N9-C1'-C2'  | -5.95 | 105.46      | 112.00   |
| 1   | CA    | 1177 | G    | N9-C1'-C2'  | -5.94 | 105.46      | 112.00   |
| 1   | CA    | 511  | C    | C2'-C3'-O3' | 5.94  | 123.21      | 113.70   |
| 1   | CA    | 27   | G    | N9-C1'-C2'  | -5.94 | 105.47      | 112.00   |
| 42  | BT    | 105  | LEU  | CA-CB-CG    | 5.94  | 128.95      | 115.30   |
| 27  | BA    | 146  | G    | C5'-C4'-C3' | -5.92 | 106.52      | 116.00   |
| 27  | DA    | 412  | A    | C5'-C4'-O4' | -5.92 | 101.99      | 109.10   |
| 27  | DA    | 2498 | C    | N1-C1'-C2'  | -5.92 | 105.48      | 112.00   |
| 38  | DP    | 54   | GLY  | N-CA-C      | -5.92 | 98.30       | 113.10   |
| 1   | AA    | 686  | U    | C2'-C3'-O3' | 5.92  | 123.16      | 113.70   |
| 27  | BA    | 474  | G    | N9-C1'-C2'  | 5.91  | 121.68      | 114.00   |
| 55  | B6    | 19   | ARG  | N-CA-C      | 5.91  | 126.96      | 111.00   |
| 27  | DA    | 313  | C    | N1-C1'-C2'  | -5.91 | 105.50      | 112.00   |
| 27  | DA    | 740  | U    | C5'-C4'-O4' | -5.90 | 102.03      | 109.10   |
| 51  | B2    | 47   | ASN  | N-CA-C      | 5.89  | 126.91      | 111.00   |
| 27  | DA    | 61   | G    | N9-C1'-C2'  | -5.88 | 105.53      | 112.00   |
| 57  | D8    | 32   | LEU  | N-CA-C      | -5.88 | 95.13       | 111.00   |
| 27  | BA    | 945  | A    | C1'-O4'-C4' | -5.88 | 105.20      | 109.90   |
| 27  | BA    | 2585 | U    | O4'-C1'-N1  | 5.87  | 112.90      | 108.20   |
| 27  | DA    | 1623 | G    | N9-C1'-C2'  | -5.87 | 105.54      | 112.00   |
| 27  | BA    | 2304 | G    | C5'-C4'-C3' | -5.87 | 106.61      | 116.00   |
| 43  | BU    | 27   | LEU  | N-CA-C      | -5.85 | 95.20       | 111.00   |
| 41  | BS    | 12   | PHE  | N-CA-C      | -5.85 | 95.21       | 111.00   |
| 1   | AA    | 723  | U    | N1-C1'-C2'  | -5.84 | 105.57      | 112.00   |
| 27  | DA    | 1653 | G    | N9-C1'-C2'  | 5.83  | 121.58      | 114.00   |
| 27  | BA    | 1744 | C    | C5'-C4'-C3' | -5.83 | 106.68      | 116.00   |
| 30  | DD    | 212  | SER  | N-CA-C      | -5.80 | 95.33       | 111.00   |
| 27  | BA    | 1784 | A    | C2'-C3'-O3' | -5.79 | 96.75       | 109.50   |
| 27  | DA    | 1929 | G    | C1'-O4'-C4' | -5.79 | 105.27      | 109.90   |
| 27  | DA    | 1236 | G    | C2'-C3'-O3' | 5.79  | 122.96      | 113.70   |
| 3   | AC    | 139  | GLN  | N-CA-C      | -5.78 | 95.39       | 111.00   |
| 27  | BA    | 906  | G    | C5'-C4'-C3' | -5.78 | 106.75      | 116.00   |
| 27  | BA    | 784  | A    | N9-C1'-C2'  | 5.78  | 121.51      | 114.00   |
| 27  | BA    | 1698 | A    | O4'-C1'-N9  | 5.77  | 112.82      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | DA    | 1698 | A    | N9-C1'-C2'  | 5.77  | 121.50      | 114.00   |
| 13  | CM    | 66   | LEU  | O-C-N       | 5.77  | 131.93      | 122.70   |
| 38  | DP    | 41   | ARG  | N-CA-C      | -5.77 | 95.43       | 111.00   |
| 28  | BB    | 40   | U    | N1-C1'-C2'  | 5.76  | 121.49      | 114.00   |
| 1   | CA    | 362  | G    | N9-C1'-C2'  | -5.76 | 105.66      | 112.00   |
| 27  | DA    | 2222 | G    | N9-C1'-C2'  | -5.76 | 105.66      | 112.00   |
| 27  | BA    | 442  | G    | N9-C1'-C2'  | 5.76  | 121.49      | 114.00   |
| 16  | AP    | 27   | LYS  | N-CA-C      | -5.76 | 95.46       | 111.00   |
| 27  | BA    | 669  | G    | N9-C1'-C2'  | 5.76  | 121.48      | 114.00   |
| 34  | BH    | 166  | GLY  | N-CA-C      | -5.75 | 98.72       | 113.10   |
| 27  | BA    | 2746 | U    | N1-C1'-C2'  | -5.75 | 105.67      | 112.00   |
| 42  | BT    | 4    | GLY  | N-CA-C      | -5.75 | 98.74       | 113.10   |
| 38  | BP    | 52   | GLU  | CA-C-N      | -5.74 | 104.72      | 116.20   |
| 1   | AA    | 957  | U    | N1-C1'-C2'  | -5.74 | 105.69      | 112.00   |
| 31  | DE    | 117  | MET  | N-CA-C      | -5.72 | 95.55       | 111.00   |
| 27  | BA    | 2200 | C    | C5'-C4'-C3' | -5.72 | 106.85      | 116.00   |
| 33  | DG    | 113  | ARG  | CA-CB-CG    | -5.71 | 100.84      | 113.40   |
| 27  | DA    | 2681 | C    | N1-C1'-C2'  | 5.71  | 121.42      | 114.00   |
| 27  | BA    | 951  | C    | N1-C1'-C2'  | -5.70 | 105.73      | 112.00   |
| 42  | BT    | 31   | SER  | N-CA-C      | 5.70  | 126.39      | 111.00   |
| 27  | BA    | 548  | A    | O4'-C1'-N9  | 5.70  | 112.76      | 108.20   |
| 1   | CA    | 960  | U    | C5'-C4'-O4' | 5.70  | 115.94      | 109.10   |
| 43  | BU    | 64   | ARG  | NE-CZ-NH2   | -5.69 | 117.45      | 120.30   |
| 27  | DA    | 2130 | U    | N1-C1'-C2'  | -5.69 | 105.74      | 112.00   |
| 57  | D8    | 32   | LEU  | CA-CB-CG    | 5.68  | 128.37      | 115.30   |
| 27  | DA    | 736  | C    | N1-C1'-C2'  | -5.68 | 105.75      | 112.00   |
| 27  | DA    | 1930 | G    | N9-C1'-C2'  | 5.68  | 121.38      | 114.00   |
| 1   | AA    | 1049 | U    | N1-C1'-C2'  | 5.68  | 121.38      | 114.00   |
| 1   | CA    | 952  | U    | N1-C1'-C2'  | -5.68 | 105.75      | 112.00   |
| 27  | DA    | 1838 | C    | C2'-C3'-O3' | 5.67  | 122.78      | 113.70   |
| 28  | BB    | 52   | A    | N9-C1'-C2'  | 5.67  | 121.37      | 114.00   |
| 1   | AA    | 428  | G    | C2'-C3'-O3' | 5.67  | 122.76      | 113.70   |
| 27  | BA    | 1517 | G    | C5'-C4'-C3' | -5.67 | 106.94      | 116.00   |
| 13  | CM    | 70   | LEU  | N-CA-CB     | 5.67  | 121.73      | 110.40   |
| 1   | AA    | 1105 | A    | N9-C1'-C2'  | -5.66 | 105.77      | 112.00   |
| 27  | BA    | 453  | C    | C5'-C4'-C3' | -5.66 | 106.94      | 116.00   |
| 41  | BS    | 26   | LEU  | N-CA-C      | -5.65 | 95.73       | 111.00   |
| 27  | BA    | 2546 | U    | O4'-C1'-N1  | 5.65  | 112.72      | 108.20   |
| 33  | BG    | 129  | GLY  | N-CA-C      | -5.65 | 98.98       | 113.10   |
| 28  | DB    | 75   | G    | C5'-C4'-C3' | -5.64 | 106.97      | 116.00   |
| 1   | AA    | 559  | A    | N9-C1'-C2'  | 5.63  | 121.32      | 114.00   |
| 27  | DA    | 1190 | G    | N9-C1'-C2'  | -5.61 | 105.83      | 112.00   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 1   | CA    | 1363(A) | A    | N9-C1'-C2'  | 5.59  | 121.27      | 114.00   |
| 1   | AA    | 400     | C    | N1-C1'-C2'  | -5.59 | 105.86      | 112.00   |
| 1   | CA    | 323     | U    | N1-C1'-C2'  | -5.58 | 105.86      | 112.00   |
| 42  | DT    | 3       | ARG  | N-CA-C      | -5.57 | 95.96       | 111.00   |
| 1   | AA    | 1274    | G    | N9-C1'-C2'  | -5.57 | 105.88      | 112.00   |
| 27  | DA    | 119     | A    | N9-C1'-C2'  | 5.57  | 121.23      | 114.00   |
| 27  | BA    | 1838    | C    | C5'-C4'-O4' | 5.56  | 115.77      | 109.10   |
| 11  | CK    | 81      | ASP  | N-CA-C      | -5.56 | 96.00       | 111.00   |
| 27  | DA    | 2092    | U    | N1-C1'-C2'  | 5.55  | 121.22      | 114.00   |
| 27  | BA    | 1204    | A    | C5'-C4'-C3' | 5.54  | 124.87      | 116.00   |
| 40  | BR    | 57      | ARG  | N-CA-C      | -5.54 | 96.04       | 111.00   |
| 41  | BS    | 16      | ASN  | N-CA-C      | -5.54 | 96.05       | 111.00   |
| 27  | DA    | 1016    | G    | N9-C1'-C2'  | -5.54 | 105.91      | 112.00   |
| 27  | DA    | 2092    | U    | C2'-C3'-O3' | 5.53  | 122.55      | 113.70   |
| 28  | BB    | 86      | G    | N9-C1'-C2'  | -5.52 | 105.93      | 112.00   |
| 27  | BA    | 934     | G    | C5'-C4'-C3' | -5.51 | 107.18      | 116.00   |
| 45  | BW    | 98      | LYS  | N-CA-C      | -5.51 | 96.12       | 111.00   |
| 27  | BA    | 1048    | A    | N9-C1'-C2'  | 5.51  | 121.16      | 114.00   |
| 27  | DA    | 2867    | G    | N9-C1'-C2'  | 5.51  | 121.16      | 114.00   |
| 27  | BA    | 2110    | G    | N9-C1'-C2'  | 5.51  | 121.16      | 114.00   |
| 4   | CD    | 31      | CYS  | N-CA-C      | -5.51 | 96.13       | 111.00   |
| 27  | DA    | 1379    | A    | C2'-C3'-O3' | 5.50  | 122.50      | 113.70   |
| 38  | BP    | 28      | GLY  | N-CA-C      | -5.49 | 99.37       | 113.10   |
| 1   | CA    | 1053    | G    | C1'-O4'-C4' | -5.49 | 105.51      | 109.90   |
| 38  | BP    | 59      | LEU  | CA-CB-CG    | 5.49  | 127.92      | 115.30   |
| 27  | DA    | 2638    | G    | C2'-C3'-O3' | 5.48  | 122.47      | 113.70   |
| 4   | CD    | 87      | GLY  | N-CA-C      | -5.48 | 99.40       | 113.10   |
| 34  | BH    | 64      | LEU  | CA-CB-CG    | -5.47 | 102.71      | 115.30   |
| 27  | BA    | 1786    | A    | N9-C1'-C2'  | 5.47  | 121.11      | 114.00   |
| 7   | AG    | 81      | GLY  | N-CA-C      | -5.47 | 99.43       | 113.10   |
| 13  | CM    | 68      | GLY  | N-CA-C      | -5.47 | 99.43       | 113.10   |
| 27  | DA    | 2304    | G    | C5'-C4'-O4' | 5.46  | 115.65      | 109.10   |
| 27  | DA    | 1799    | G    | N9-C1'-C2'  | 5.46  | 121.10      | 114.00   |
| 40  | BR    | 60      | LEU  | CA-CB-CG    | 5.45  | 127.84      | 115.30   |
| 40  | BR    | 4       | LEU  | N-CA-C      | 5.45  | 125.72      | 111.00   |
| 27  | BA    | 670     | A    | C2'-C3'-O3' | 5.45  | 122.42      | 113.70   |
| 1   | AA    | 1134    | G    | N9-C1'-C2'  | -5.45 | 106.01      | 112.00   |
| 1   | CA    | 517     | G    | C4'-C3'-O3' | 5.45  | 123.90      | 113.00   |
| 1   | AA    | 108     | G    | O4'-C1'-N9  | 5.45  | 112.56      | 108.20   |
| 27  | BA    | 1815    | A    | N9-C1'-C2'  | 5.45  | 121.08      | 114.00   |
| 41  | DS    | 17      | ARG  | N-CA-C      | -5.45 | 96.30       | 111.00   |
| 1   | CA    | 1201    | A    | C2'-C3'-O3' | 5.44  | 122.41      | 113.70   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 33  | DG    | 113     | ARG  | CA-C-N      | -5.44 | 105.23      | 117.20   |
| 1   | CA    | 994     | A    | N9-C1'-C2'  | -5.44 | 106.02      | 112.00   |
| 42  | BT    | 35      | LYS  | N-CA-C      | -5.43 | 96.32       | 111.00   |
| 13  | CM    | 66      | LEU  | CA-CB-CG    | 5.42  | 127.77      | 115.30   |
| 27  | DA    | 157     | U    | N1-C1'-C2'  | 5.41  | 121.04      | 114.00   |
| 27  | DA    | 2419    | U    | N1-C1'-C2'  | -5.41 | 106.05      | 112.00   |
| 27  | DA    | 2585    | U    | N1-C1'-C2'  | 5.41  | 121.04      | 114.00   |
| 1   | CA    | 699     | C    | N1-C1'-C2'  | -5.41 | 106.05      | 112.00   |
| 27  | DA    | 125     | G    | N9-C1'-C2'  | 5.40  | 121.02      | 114.00   |
| 1   | AA    | 1442(A) | G    | O4'-C1'-N9  | 5.39  | 112.51      | 108.20   |
| 27  | DA    | 40      | C    | N1-C1'-C2'  | -5.39 | 106.07      | 112.00   |
| 27  | DA    | 1963    | U    | N1-C1'-C2'  | 5.39  | 121.01      | 114.00   |
| 27  | BA    | 572     | A    | O5'-P-OP2   | -5.39 | 100.85      | 105.70   |
| 27  | DA    | 2832    | U    | C2'-C3'-O3' | 5.39  | 122.32      | 113.70   |
| 27  | BA    | 717     | G    | N9-C1'-C2'  | -5.39 | 106.08      | 112.00   |
| 27  | BA    | 1033    | U    | OP1-P-O3'   | 5.38  | 117.03      | 105.20   |
| 27  | BA    | 2873    | A    | O4'-C1'-N9  | 5.37  | 112.50      | 108.20   |
| 55  | D6    | 19      | ARG  | N-CA-C      | 5.37  | 125.49      | 111.00   |
| 1   | AA    | 1442(A) | G    | C2'-C3'-O3' | -5.37 | 97.70       | 109.50   |
| 27  | BA    | 2042    | A    | N9-C1'-C2'  | -5.35 | 106.11      | 112.00   |
| 33  | BG    | 87      | PRO  | N-CA-C      | 5.35  | 126.02      | 112.10   |
| 28  | DB    | 35      | U    | N1-C1'-C2'  | -5.35 | 106.11      | 112.00   |
| 1   | AA    | 154     | C    | N1-C1'-C2'  | -5.35 | 106.11      | 112.00   |
| 27  | BA    | 1559    | G    | O4'-C1'-N9  | 5.35  | 112.48      | 108.20   |
| 27  | BA    | 1175    | U    | N1-C1'-C2'  | 5.35  | 120.95      | 114.00   |
| 47  | BY    | 54      | LYS  | N-CA-C      | -5.34 | 96.58       | 111.00   |
| 27  | BA    | 1772    | G    | N9-C1'-C2'  | -5.34 | 106.13      | 112.00   |
| 27  | DA    | 2021    | C    | OP1-P-O3'   | 5.34  | 116.95      | 105.20   |
| 27  | DA    | 2440    | C    | O4'-C1'-N1  | 5.34  | 112.47      | 108.20   |
| 27  | DA    | 1460    | A    | C2'-C3'-O3' | 5.34  | 122.24      | 113.70   |
| 1   | AA    | 189(I)  | G    | N9-C1'-C2'  | -5.34 | 106.13      | 112.00   |
| 43  | DU    | 9       | VAL  | N-CA-C      | 5.33  | 125.39      | 111.00   |
| 1   | AA    | 1380    | U    | N1-C1'-C2'  | 5.33  | 120.92      | 114.00   |
| 27  | DA    | 2276    | G    | N9-C1'-C2'  | -5.32 | 106.15      | 112.00   |
| 27  | BA    | 1139    | G    | N9-C1'-C2'  | -5.32 | 106.15      | 112.00   |
| 27  | DA    | 271(D)  | G    | N9-C1'-C2'  | -5.32 | 106.15      | 112.00   |
| 27  | BA    | 629     | G    | C5'-C4'-C3' | -5.31 | 107.50      | 116.00   |
| 27  | DA    | 2702    | U    | N1-C1'-C2'  | 5.31  | 120.90      | 114.00   |
| 44  | BV    | 39      | LEU  | CA-CB-CG    | 5.30  | 127.49      | 115.30   |
| 27  | BA    | 2672    | G    | C5'-C4'-C3' | -5.30 | 107.52      | 116.00   |
| 27  | BA    | 945     | A    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 54  | B5    | 3       | LYS  | N-CA-C      | 5.30  | 125.30      | 111.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 43  | DU    | 97   | ASP  | N-CA-C      | -5.30 | 96.70       | 111.00   |
| 1   | CA    | 890  | G    | N9-C1'-C2'  | 5.29  | 120.88      | 114.00   |
| 27  | BA    | 454  | A    | OP1-P-O3'   | 5.29  | 116.83      | 105.20   |
| 44  | BV    | 37   | VAL  | N-CA-C      | -5.28 | 96.74       | 111.00   |
| 1   | CA    | 429  | U    | O4'-C1'-N1  | 5.27  | 112.42      | 108.20   |
| 27  | DA    | 2060 | A    | C2'-C3'-O3' | 5.27  | 122.13      | 113.70   |
| 27  | DA    | 2140 | C    | N1-C1'-C2'  | -5.27 | 106.20      | 112.00   |
| 1   | AA    | 1064 | G    | C2'-C3'-O3' | 5.27  | 122.13      | 113.70   |
| 27  | BA    | 11   | G    | N9-C1'-C2'  | -5.26 | 106.21      | 112.00   |
| 40  | BR    | 6    | SER  | N-CA-C      | 5.26  | 125.21      | 111.00   |
| 1   | CA    | 328  | C    | N1-C1'-C2'  | 5.26  | 120.84      | 114.00   |
| 27  | DA    | 469  | G    | N9-C1'-C2'  | -5.26 | 106.21      | 112.00   |
| 27  | DA    | 742  | G    | N9-C1'-C2'  | -5.25 | 106.22      | 112.00   |
| 1   | AA    | 1174 | G    | N9-C1'-C2'  | -5.25 | 106.23      | 112.00   |
| 36  | BN    | 124  | ALA  | N-CA-C      | -5.25 | 96.84       | 111.00   |
| 1   | CA    | 723  | U    | N1-C1'-C2'  | -5.24 | 106.23      | 112.00   |
| 27  | DA    | 33   | U    | C1'-O4'-C4' | -5.24 | 105.70      | 109.90   |
| 27  | DA    | 1165 | U    | N1-C1'-C2'  | -5.24 | 106.23      | 112.00   |
| 27  | BA    | 1308 | A    | N9-C1'-C2'  | -5.24 | 106.24      | 112.00   |
| 27  | DA    | 1914 | C    | O4'-C1'-N1  | 5.24  | 112.39      | 108.20   |
| 1   | AA    | 533  | A    | C2'-C3'-O3' | 5.24  | 122.08      | 113.70   |
| 1   | CA    | 1141 | C    | N1-C1'-C2'  | 5.24  | 120.81      | 114.00   |
| 47  | BY    | 47   | LYS  | N-CA-C      | 5.23  | 125.13      | 111.00   |
| 37  | BO    | 59   | LYS  | N-CA-C      | -5.22 | 96.90       | 111.00   |
| 1   | CA    | 454  | C    | O4'-C1'-N1  | 5.22  | 112.38      | 108.20   |
| 4   | AD    | 12   | CYS  | N-CA-C      | -5.22 | 96.91       | 111.00   |
| 27  | BA    | 2231 | C    | N1-C1'-C2'  | -5.21 | 106.27      | 112.00   |
| 57  | D8    | 38   | GLY  | N-CA-C      | -5.21 | 100.07      | 113.10   |
| 13  | CM    | 70   | LEU  | CA-CB-CG    | -5.21 | 103.32      | 115.30   |
| 27  | BA    | 2699 | C    | N1-C1'-C2'  | -5.21 | 106.27      | 112.00   |
| 27  | DA    | 790  | C    | N1-C1'-C2'  | 5.20  | 120.77      | 114.00   |
| 27  | DA    | 284  | U    | N1-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 27  | DA    | 779  | U    | N1-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 37  | BO    | 40   | VAL  | N-CA-C      | -5.20 | 96.96       | 111.00   |
| 27  | DA    | 1936 | A    | C1'-O4'-C4' | -5.20 | 105.74      | 109.90   |
| 27  | BA    | 2712 | U    | C5'-C4'-O4' | 5.20  | 115.33      | 109.10   |
| 22  | CV    | 6    | G    | N9-C1'-C2'  | 5.19  | 120.75      | 114.00   |
| 1   | AA    | 1020 | U    | N1-C1'-C2'  | -5.19 | 106.29      | 112.00   |
| 1   | AA    | 181  | G    | C5'-C4'-O4' | 5.19  | 115.32      | 109.10   |
| 27  | DA    | 1321 | A    | C5'-C4'-C3' | -5.18 | 107.71      | 116.00   |
| 1   | AA    | 351  | G    | N9-C1'-C2'  | 5.17  | 120.73      | 114.00   |
| 27  | DA    | 676  | A    | C1'-O4'-C4' | -5.17 | 105.76      | 109.90   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | AA    | 770    | C    | N1-C1'-C2'  | -5.17 | 106.31      | 112.00   |
| 27  | DA    | 474    | G    | N9-C1'-C2'  | 5.17  | 120.72      | 114.00   |
| 1   | AA    | 1530   | G    | N9-C1'-C2'  | -5.16 | 106.32      | 112.00   |
| 1   | CA    | 401    | C    | N1-C1'-C2'  | -5.16 | 106.32      | 112.00   |
| 27  | BA    | 1126   | A    | C4'-C3'-C2' | 5.16  | 107.76      | 102.60   |
| 27  | BA    | 2712   | U    | O4'-C1'-N1  | 5.16  | 112.33      | 108.20   |
| 38  | BP    | 27     | HIS  | N-CA-C      | 5.16  | 124.93      | 111.00   |
| 1   | AA    | 1124   | G    | N9-C1'-C2'  | 5.16  | 120.70      | 114.00   |
| 27  | BA    | 2682   | U    | C5'-C4'-O4' | -5.15 | 102.92      | 109.10   |
| 27  | DA    | 2712   | U    | O4'-C1'-N1  | 5.15  | 112.32      | 108.20   |
| 27  | BA    | 349    | G    | C5'-C4'-C3' | -5.15 | 107.77      | 116.00   |
| 56  | B7    | 42     | LEU  | CA-CB-CG    | 5.14  | 127.13      | 115.30   |
| 27  | BA    | 2447   | G    | C5'-C4'-O4' | -5.14 | 102.93      | 109.10   |
| 27  | DA    | 2286   | A    | N9-C1'-C2'  | 5.14  | 120.68      | 114.00   |
| 27  | BA    | 272(B) | G    | C5'-C4'-C3' | 5.13  | 124.20      | 116.00   |
| 27  | BA    | 2092   | U    | N1-C1'-C2'  | 5.12  | 120.66      | 114.00   |
| 1   | AA    | 872    | A    | N9-C1'-C2'  | 5.12  | 120.65      | 114.00   |
| 27  | BA    | 310    | A    | C1'-O4'-C4' | -5.12 | 105.81      | 109.90   |
| 32  | DF    | 85     | GLY  | N-CA-C      | -5.12 | 100.31      | 113.10   |
| 27  | BA    | 493    | G    | C5'-C4'-C3' | -5.11 | 107.82      | 116.00   |
| 27  | DA    | 671    | C    | N1-C1'-C2'  | -5.11 | 106.38      | 112.00   |
| 27  | BA    | 748    | G    | N9-C1'-C2'  | 5.11  | 120.64      | 114.00   |
| 27  | BA    | 142    | A    | N9-C1'-C2'  | 5.10  | 120.64      | 114.00   |
| 27  | BA    | 343    | C    | C5'-C4'-C3' | -5.09 | 107.85      | 116.00   |
| 30  | DD    | 259    | THR  | N-CA-C      | 5.09  | 124.75      | 111.00   |
| 47  | DY    | 99     | CYS  | CA-CB-SG    | 5.09  | 123.17      | 114.00   |
| 30  | BD    | 241    | PRO  | N-CA-C      | 5.09  | 125.34      | 112.10   |
| 47  | BY    | 59     | GLY  | N-CA-C      | 5.09  | 125.82      | 113.10   |
| 1   | CA    | 356    | A    | N9-C1'-C2'  | -5.09 | 106.40      | 112.00   |
| 40  | BR    | 70     | LEU  | N-CA-C      | -5.09 | 97.26       | 111.00   |
| 40  | DR    | 5      | LYS  | N-CA-C      | -5.09 | 97.26       | 111.00   |
| 45  | BW    | 102    | HIS  | N-CA-C      | -5.08 | 97.28       | 111.00   |
| 1   | CA    | 781    | A    | N9-C1'-C2'  | -5.08 | 106.41      | 112.00   |
| 27  | DA    | 242    | G    | N9-C1'-C2'  | 5.07  | 120.59      | 114.00   |
| 27  | DA    | 1360   | A    | C5'-C4'-C3' | -5.07 | 107.89      | 116.00   |
| 27  | BA    | 1272   | A    | C5'-C4'-O4' | 5.07  | 115.18      | 109.10   |
| 27  | DA    | 1775   | U    | N1-C1'-C2'  | -5.06 | 106.43      | 112.00   |
| 42  | DT    | 30     | VAL  | N-CA-C      | 5.06  | 124.67      | 111.00   |
| 27  | DA    | 1034   | G    | N9-C1'-C2'  | -5.06 | 106.43      | 112.00   |
| 13  | CM    | 113    | PRO  | CA-N-CD     | -5.06 | 104.42      | 111.50   |
| 27  | DA    | 1015   | G    | C5'-C4'-C3' | -5.06 | 107.91      | 116.00   |
| 33  | BG    | 88     | ILE  | N-CA-C      | 5.06  | 124.66      | 111.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | DX    | 57   | LEU  | CA-CB-CG    | 5.06  | 126.93      | 115.30   |
| 27  | BA    | 1051 | G    | N9-C1'-C2'  | -5.05 | 106.45      | 112.00   |
| 37  | BO    | 50   | GLY  | N-CA-C      | 5.05  | 125.72      | 113.10   |
| 11  | AK    | 86   | GLY  | N-CA-C      | 5.04  | 125.71      | 113.10   |
| 55  | D6    | 46   | HIS  | O-C-N       | 5.04  | 130.77      | 122.70   |
| 27  | BA    | 2879 | C    | OP1-P-O3'   | 5.04  | 116.29      | 105.20   |
| 33  | BG    | 113  | ARG  | CA-C-N      | -5.04 | 106.11      | 117.20   |
| 27  | DA    | 119  | A    | C2'-C3'-O3' | 5.04  | 121.76      | 113.70   |
| 37  | BO    | 51   | ALA  | N-CA-C      | -5.03 | 97.41       | 111.00   |
| 30  | DD    | 68   | LYS  | N-CA-C      | -5.03 | 97.41       | 111.00   |
| 1   | CA    | 1380 | U    | C2'-C3'-O3' | 5.03  | 121.74      | 113.70   |
| 55  | B6    | 48   | VAL  | N-CA-C      | 5.03  | 124.57      | 111.00   |
| 27  | DA    | 2021 | C    | N1-C1'-C2'  | 5.02  | 120.52      | 114.00   |
| 14  | CN    | 40   | CYS  | N-CA-C      | -5.01 | 97.46       | 111.00   |
| 1   | CA    | 974  | A    | N9-C1'-C2'  | 5.01  | 120.52      | 114.00   |
| 28  | DB    | 84   | C    | N1-C1'-C2'  | -5.01 | 106.49      | 112.00   |
| 44  | BV    | 49   | THR  | N-CA-C      | -5.01 | 97.48       | 111.00   |
| 27  | DA    | 656  | G    | O4'-C1'-N9  | 5.01  | 112.21      | 108.20   |
| 27  | BA    | 1862 | G    | N9-C1'-C2'  | -5.00 | 106.50      | 112.00   |
| 27  | DA    | 797  | C    | N1-C1'-C2'  | -5.00 | 106.50      | 112.00   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | CA    | 517 | G    | C3'  |

All (582) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1000 | U    | Sidechain |
| 1   | AA    | 1020 | U    | Sidechain |
| 1   | AA    | 1040 | U    | Sidechain |
| 1   | AA    | 1060 | C    | Sidechain |
| 1   | AA    | 1062 | U    | Sidechain |
| 1   | AA    | 1073 | U    | Sidechain |
| 1   | AA    | 1076 | C    | Sidechain |
| 1   | AA    | 1077 | G    | Sidechain |
| 1   | AA    | 1085 | U    | Sidechain |
| 1   | AA    | 1101 | A    | Sidechain |
| 1   | AA    | 1124 | G    | Sidechain |
| 1   | AA    | 115  | G    | Sidechain |
| 1   | AA    | 1152 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1198 | G    | Sidechain |
| 1   | AA    | 12   | U    | Sidechain |
| 1   | AA    | 1225 | A    | Sidechain |
| 1   | AA    | 1264 | C    | Sidechain |
| 1   | AA    | 1279 | A    | Sidechain |
| 1   | AA    | 1309 | G    | Sidechain |
| 1   | AA    | 131  | C    | Sidechain |
| 1   | AA    | 1314 | C    | Sidechain |
| 1   | AA    | 142  | G    | Sidechain |
| 1   | AA    | 1437 | C    | Sidechain |
| 1   | AA    | 1461 | G    | Sidechain |
| 1   | AA    | 1472 | U    | Sidechain |
| 1   | AA    | 1505 | G    | Sidechain |
| 1   | AA    | 151  | A    | Sidechain |
| 1   | AA    | 1519 | A    | Sidechain |
| 1   | AA    | 1530 | G    | Sidechain |
| 1   | AA    | 154  | C    | Sidechain |
| 1   | AA    | 17   | U    | Sidechain |
| 1   | AA    | 182  | U    | Sidechain |
| 1   | AA    | 190  | U    | Sidechain |
| 1   | AA    | 198  | G    | Sidechain |
| 1   | AA    | 240  | C    | Sidechain |
| 1   | AA    | 253  | U    | Sidechain |
| 1   | AA    | 287  | U    | Sidechain |
| 1   | AA    | 290  | C    | Sidechain |
| 1   | AA    | 297  | G    | Sidechain |
| 1   | AA    | 315  | A    | Sidechain |
| 1   | AA    | 34   | C    | Sidechain |
| 1   | AA    | 343  | U    | Sidechain |
| 1   | AA    | 365  | U    | Sidechain |
| 1   | AA    | 372  | C    | Sidechain |
| 1   | AA    | 425  | G    | Sidechain |
| 1   | AA    | 438  | G    | Sidechain |
| 1   | AA    | 450  | G    | Sidechain |
| 1   | AA    | 461  | A    | Sidechain |
| 1   | AA    | 470  | C    | Sidechain |
| 1   | AA    | 471  | G    | Sidechain |
| 1   | AA    | 484  | G    | Sidechain |
| 1   | AA    | 486  | U    | Sidechain |
| 1   | AA    | 49   | U    | Sidechain |
| 1   | AA    | 498  | U    | Sidechain |
| 1   | AA    | 508  | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 512  | U    | Sidechain |
| 1   | AA    | 518  | C    | Sidechain |
| 1   | AA    | 52   | G    | Sidechain |
| 1   | AA    | 528  | C    | Sidechain |
| 1   | AA    | 534  | U    | Sidechain |
| 1   | AA    | 545  | C    | Sidechain |
| 1   | AA    | 577  | G    | Sidechain |
| 1   | AA    | 578  | C    | Sidechain |
| 1   | AA    | 603  | U    | Sidechain |
| 1   | AA    | 657  | G    | Sidechain |
| 1   | AA    | 664  | G    | Sidechain |
| 1   | AA    | 669  | U    | Sidechain |
| 1   | AA    | 672  | U    | Sidechain |
| 1   | AA    | 678  | U    | Sidechain |
| 1   | AA    | 682  | G    | Sidechain |
| 1   | AA    | 688  | G    | Sidechain |
| 1   | AA    | 697  | U    | Sidechain |
| 1   | AA    | 700  | G    | Sidechain |
| 1   | AA    | 721  | G    | Sidechain |
| 1   | AA    | 723  | U    | Sidechain |
| 1   | AA    | 729  | A    | Sidechain |
| 1   | AA    | 752  | G    | Sidechain |
| 1   | AA    | 775  | G    | Sidechain |
| 1   | AA    | 793  | U    | Sidechain |
| 1   | AA    | 801  | U    | Sidechain |
| 1   | AA    | 837  | G    | Sidechain |
| 1   | AA    | 879  | C    | Sidechain |
| 1   | AA    | 882  | C    | Sidechain |
| 1   | AA    | 890  | G    | Sidechain |
| 1   | AA    | 897  | C    | Sidechain |
| 1   | AA    | 936  | C    | Sidechain |
| 1   | AA    | 940  | C    | Sidechain |
| 1   | AA    | 974  | A    | Sidechain |
| 1   | AA    | 981  | U    | Sidechain |
| 1   | AA    | 984  | C    | Sidechain |
| 23  | AW    | 34   | U    | Sidechain |
| 55  | B6    | 46   | HIS  | Sidechain |
| 27  | BA    | 1007 | C    | Sidechain |
| 27  | BA    | 1017 | G    | Sidechain |
| 27  | BA    | 1021 | A    | Sidechain |
| 27  | BA    | 1025 | G    | Sidechain |
| 27  | BA    | 1048 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 27  | BA    | 1051 | G    | Sidechain |
| 27  | BA    | 1121 | C    | Sidechain |
| 27  | BA    | 1130 | U    | Sidechain |
| 27  | BA    | 1133 | U    | Sidechain |
| 27  | BA    | 1139 | G    | Sidechain |
| 27  | BA    | 1140 | C    | Sidechain |
| 27  | BA    | 1143 | A    | Sidechain |
| 27  | BA    | 1192 | G    | Sidechain |
| 27  | BA    | 120  | U    | Sidechain |
| 27  | BA    | 1205 | U    | Sidechain |
| 27  | BA    | 1215 | G    | Sidechain |
| 27  | BA    | 1225 | G    | Sidechain |
| 27  | BA    | 1231 | G    | Sidechain |
| 27  | BA    | 1253 | A    | Sidechain |
| 27  | BA    | 1265 | A    | Sidechain |
| 27  | BA    | 1271 | G    | Sidechain |
| 27  | BA    | 1283 | G    | Sidechain |
| 27  | BA    | 1288 | U    | Sidechain |
| 27  | BA    | 1300 | U    | Sidechain |
| 27  | BA    | 1308 | A    | Sidechain |
| 27  | BA    | 1309 | G    | Sidechain |
| 27  | BA    | 1310 | G    | Sidechain |
| 27  | BA    | 1323 | U    | Sidechain |
| 27  | BA    | 1349 | A    | Sidechain |
| 27  | BA    | 1364 | G    | Sidechain |
| 27  | BA    | 1379 | A    | Sidechain |
| 27  | BA    | 1391 | U    | Sidechain |
| 27  | BA    | 1396 | U    | Sidechain |
| 27  | BA    | 140  | G    | Sidechain |
| 27  | BA    | 1405 | U    | Sidechain |
| 27  | BA    | 1410 | G    | Sidechain |
| 27  | BA    | 1425 | G    | Sidechain |
| 27  | BA    | 1428 | C    | Sidechain |
| 27  | BA    | 1433 | U    | Sidechain |
| 27  | BA    | 1437 | C    | Sidechain |
| 27  | BA    | 1451 | C    | Sidechain |
| 27  | BA    | 1497 | U    | Sidechain |
| 27  | BA    | 15   | G    | Sidechain |
| 27  | BA    | 1603 | A    | Sidechain |
| 27  | BA    | 1620 | G    | Sidechain |
| 27  | BA    | 1630 | G    | Sidechain |
| 27  | BA    | 1659 | U    | Sidechain |

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| Mol | Chain | Res     | Type | Group     |
|-----|-------|---------|------|-----------|
| 27  | BA    | 1680    | U    | Sidechain |
| 27  | BA    | 1704    | G    | Sidechain |
| 27  | BA    | 1709    | U    | Sidechain |
| 27  | BA    | 1742    | G    | Sidechain |
| 27  | BA    | 1745(A) | C    | Sidechain |
| 27  | BA    | 1772    | G    | Sidechain |
| 27  | BA    | 1775    | U    | Sidechain |
| 27  | BA    | 1779    | U    | Sidechain |
| 27  | BA    | 1780    | A    | Sidechain |
| 27  | BA    | 1783    | A    | Sidechain |
| 27  | BA    | 1784    | A    | Sidechain |
| 27  | BA    | 1796    | U    | Sidechain |
| 27  | BA    | 1861    | G    | Sidechain |
| 27  | BA    | 1884    | A    | Sidechain |
| 27  | BA    | 1903    | G    | Sidechain |
| 27  | BA    | 1915    | U    | Sidechain |
| 27  | BA    | 1935    | G    | Sidechain |
| 27  | BA    | 1938    | A    | Sidechain |
| 27  | BA    | 1952    | A    | Sidechain |
| 27  | BA    | 1976    | U    | Sidechain |
| 27  | BA    | 1978    | A    | Sidechain |
| 27  | BA    | 1983    | C    | Sidechain |
| 27  | BA    | 1984    | G    | Sidechain |
| 27  | BA    | 1996    | C    | Sidechain |
| 27  | BA    | 1998    | G    | Sidechain |
| 27  | BA    | 1999    | C    | Sidechain |
| 27  | BA    | 2000    | G    | Sidechain |
| 27  | BA    | 2010    | G    | Sidechain |
| 27  | BA    | 2022    | U    | Sidechain |
| 27  | BA    | 2032    | G    | Sidechain |
| 27  | BA    | 2036    | C    | Sidechain |
| 27  | BA    | 2041    | U    | Sidechain |
| 27  | BA    | 2053    | G    | Sidechain |
| 27  | BA    | 2068    | U    | Sidechain |
| 27  | BA    | 2074    | U    | Sidechain |
| 27  | BA    | 2086    | U    | Sidechain |
| 27  | BA    | 2110    | G    | Sidechain |
| 27  | BA    | 2126    | A    | Sidechain |
| 27  | BA    | 2127    | G    | Sidechain |
| 27  | BA    | 22      | C    | Sidechain |
| 27  | BA    | 223     | A    | Sidechain |
| 27  | BA    | 2232    | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 27  | BA    | 2233 | U    | Sidechain |
| 27  | BA    | 2243 | U    | Sidechain |
| 27  | BA    | 2249 | U    | Sidechain |
| 27  | BA    | 226  | G    | Sidechain |
| 27  | BA    | 2308 | G    | Sidechain |
| 27  | BA    | 2319 | G    | Sidechain |
| 27  | BA    | 2335 | A    | Sidechain |
| 27  | BA    | 2344 | U    | Sidechain |
| 27  | BA    | 235  | U    | Sidechain |
| 27  | BA    | 2370 | G    | Sidechain |
| 27  | BA    | 2375 | G    | Sidechain |
| 27  | BA    | 2390 | U    | Sidechain |
| 27  | BA    | 2401 | U    | Sidechain |
| 27  | BA    | 2406 | U    | Sidechain |
| 27  | BA    | 2424 | C    | Sidechain |
| 27  | BA    | 2437 | U    | Sidechain |
| 27  | BA    | 2461 | C    | Sidechain |
| 27  | BA    | 2475 | C    | Sidechain |
| 27  | BA    | 2477 | C    | Sidechain |
| 27  | BA    | 2481 | G    | Sidechain |
| 27  | BA    | 2484 | G    | Sidechain |
| 27  | BA    | 2486 | G    | Sidechain |
| 27  | BA    | 249  | C    | Sidechain |
| 27  | BA    | 2491 | U    | Sidechain |
| 27  | BA    | 2504 | U    | Sidechain |
| 27  | BA    | 2511 | U    | Sidechain |
| 27  | BA    | 2519 | U    | Sidechain |
| 27  | BA    | 2522 | U    | Sidechain |
| 27  | BA    | 2523 | G    | Sidechain |
| 27  | BA    | 2524 | G    | Sidechain |
| 27  | BA    | 2525 | G    | Sidechain |
| 27  | BA    | 2529 | G    | Sidechain |
| 27  | BA    | 2542 | A    | Sidechain |
| 27  | BA    | 2554 | U    | Sidechain |
| 27  | BA    | 2555 | U    | Sidechain |
| 27  | BA    | 2558 | C    | Sidechain |
| 27  | BA    | 256  | A    | Sidechain |
| 27  | BA    | 2574 | G    | Sidechain |
| 27  | BA    | 2589 | A    | Sidechain |
| 27  | BA    | 2595 | G    | Sidechain |
| 27  | BA    | 2597 | G    | Sidechain |
| 27  | BA    | 2606 | C    | Sidechain |

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| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 27  | BA    | 2607   | G    | Sidechain |
| 27  | BA    | 2608   | G    | Sidechain |
| 27  | BA    | 2609   | U    | Sidechain |
| 27  | BA    | 2636   | U    | Sidechain |
| 27  | BA    | 2640   | G    | Sidechain |
| 27  | BA    | 2689   | U    | Sidechain |
| 27  | BA    | 2692   | C    | Sidechain |
| 27  | BA    | 271(D) | G    | Sidechain |
| 27  | BA    | 271(E) | U    | Sidechain |
| 27  | BA    | 271(K) | U    | Sidechain |
| 27  | BA    | 2712   | U    | Sidechain |
| 27  | BA    | 2720   | U    | Sidechain |
| 27  | BA    | 2724   | C    | Sidechain |
| 27  | BA    | 2739   | U    | Sidechain |
| 27  | BA    | 2778   | A    | Sidechain |
| 27  | BA    | 2779   | U    | Sidechain |
| 27  | BA    | 2832   | U    | Sidechain |
| 27  | BA    | 2836   | U    | Sidechain |
| 27  | BA    | 2846   | G    | Sidechain |
| 27  | BA    | 2857   | G    | Sidechain |
| 27  | BA    | 2866   | U    | Sidechain |
| 27  | BA    | 2872   | G    | Sidechain |
| 27  | BA    | 2873   | A    | Sidechain |
| 27  | BA    | 2875   | C    | Sidechain |
| 27  | BA    | 2884   | U    | Sidechain |
| 27  | BA    | 2885   | C    | Sidechain |
| 27  | BA    | 2887   | U    | Sidechain |
| 27  | BA    | 301    | G    | Sidechain |
| 27  | BA    | 326    | G    | Sidechain |
| 27  | BA    | 34     | C    | Sidechain |
| 27  | BA    | 340    | A    | Sidechain |
| 27  | BA    | 363(E) | U    | Sidechain |
| 27  | BA    | 373    | U    | Sidechain |
| 27  | BA    | 387    | U    | Sidechain |
| 27  | BA    | 390    | A    | Sidechain |
| 27  | BA    | 396    | G    | Sidechain |
| 27  | BA    | 403    | U    | Sidechain |
| 27  | BA    | 434    | U    | Sidechain |
| 27  | BA    | 436    | C    | Sidechain |
| 27  | BA    | 44     | G    | Sidechain |
| 27  | BA    | 463    | G    | Sidechain |
| 27  | BA    | 467    | G    | Sidechain |

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| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 27  | BA    | 47     | C    | Sidechain |
| 27  | BA    | 479    | A    | Sidechain |
| 27  | BA    | 511    | U    | Sidechain |
| 27  | BA    | 562    | U    | Sidechain |
| 27  | BA    | 607    | U    | Sidechain |
| 27  | BA    | 61     | G    | Sidechain |
| 27  | BA    | 614    | U    | Sidechain |
| 27  | BA    | 614(A) | U    | Sidechain |
| 27  | BA    | 628    | G    | Sidechain |
| 27  | BA    | 630    | G    | Sidechain |
| 27  | BA    | 648    | G    | Sidechain |
| 27  | BA    | 652    | C    | Sidechain |
| 27  | BA    | 657    | U    | Sidechain |
| 27  | BA    | 661    | C    | Sidechain |
| 27  | BA    | 663    | G    | Sidechain |
| 27  | BA    | 668    | G    | Sidechain |
| 27  | BA    | 674    | G    | Sidechain |
| 27  | BA    | 695    | G    | Sidechain |
| 27  | BA    | 715    | G    | Sidechain |
| 27  | BA    | 725    | G    | Sidechain |
| 27  | BA    | 742    | G    | Sidechain |
| 27  | BA    | 743    | G    | Sidechain |
| 27  | BA    | 750    | A    | Sidechain |
| 27  | BA    | 77     | C    | Sidechain |
| 27  | BA    | 777    | A    | Sidechain |
| 27  | BA    | 787    | U    | Sidechain |
| 27  | BA    | 808    | G    | Sidechain |
| 27  | BA    | 827    | U    | Sidechain |
| 27  | BA    | 834    | C    | Sidechain |
| 27  | BA    | 842    | G    | Sidechain |
| 27  | BA    | 847    | U    | Sidechain |
| 27  | BA    | 859    | G    | Sidechain |
| 27  | BA    | 868    | U    | Sidechain |
| 27  | BA    | 871    | U    | Sidechain |
| 27  | BA    | 88     | G    | Sidechain |
| 27  | BA    | 90     | U    | Sidechain |
| 27  | BA    | 916    | G    | Sidechain |
| 27  | BA    | 928    | G    | Sidechain |
| 27  | BA    | 937    | U    | Sidechain |
| 27  | BA    | 943    | U    | Sidechain |
| 27  | BA    | 947    | G    | Sidechain |
| 27  | BA    | 950    | G    | Sidechain |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 27         | BA           | 951        | C           | Sidechain    |
| 27         | BA           | 956        | G           | Sidechain    |
| 27         | BA           | 958        | U           | Sidechain    |
| 27         | BA           | 959        | A           | Sidechain    |
| 27         | BA           | 964        | C           | Sidechain    |
| 27         | BA           | 985        | C           | Sidechain    |
| 27         | BA           | 996        | A           | Sidechain    |
| 27         | BA           | 999        | U           | Sidechain    |
| 28         | BB           | 1          | U           | Sidechain    |
| 28         | BB           | 105        | A           | Sidechain    |
| 28         | BB           | 118        | G           | Sidechain    |
| 28         | BB           | 12         | C           | Sidechain    |
| 28         | BB           | 40         | U           | Sidechain    |
| 28         | BB           | 66         | A           | Sidechain    |
| 47         | BY           | 55         | TYR         | Sidechain    |
| 1          | CA           | 1052       | U           | Sidechain    |
| 1          | CA           | 1055       | A           | Sidechain    |
| 1          | CA           | 106        | C           | Sidechain    |
| 1          | CA           | 1077       | G           | Sidechain    |
| 1          | CA           | 1122       | U           | Sidechain    |
| 1          | CA           | 1140       | C           | Sidechain    |
| 1          | CA           | 1160       | G           | Sidechain    |
| 1          | CA           | 1177       | G           | Sidechain    |
| 1          | CA           | 1217       | C           | Sidechain    |
| 1          | CA           | 1225       | A           | Sidechain    |
| 1          | CA           | 1226       | C           | Sidechain    |
| 1          | CA           | 1240       | U           | Sidechain    |
| 1          | CA           | 1282       | C           | Sidechain    |
| 1          | CA           | 1289       | A           | Sidechain    |
| 1          | CA           | 1293       | G           | Sidechain    |
| 1          | CA           | 13         | U           | Sidechain    |
| 1          | CA           | 1302       | U           | Sidechain    |
| 1          | CA           | 131        | C           | Sidechain    |
| 1          | CA           | 1316       | G           | Sidechain    |
| 1          | CA           | 133        | U           | Sidechain    |
| 1          | CA           | 1331       | G           | Sidechain    |
| 1          | CA           | 1351       | U           | Sidechain    |
| 1          | CA           | 1363(A)    | A           | Sidechain    |
| 1          | CA           | 1405       | G           | Sidechain    |
| 1          | CA           | 1498       | U           | Sidechain    |
| 1          | CA           | 1504       | G           | Sidechain    |
| 1          | CA           | 1506       | U           | Sidechain    |

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| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 1   | CA    | 182    | U    | Sidechain |
| 1   | CA    | 189(G) | G    | Sidechain |
| 1   | CA    | 195    | A    | Sidechain |
| 1   | CA    | 199    | G    | Sidechain |
| 1   | CA    | 21     | G    | Sidechain |
| 1   | CA    | 245    | C    | Sidechain |
| 1   | CA    | 246    | A    | Sidechain |
| 1   | CA    | 250    | A    | Sidechain |
| 1   | CA    | 253    | U    | Sidechain |
| 1   | CA    | 266    | G    | Sidechain |
| 1   | CA    | 277    | C    | Sidechain |
| 1   | CA    | 279    | A    | Sidechain |
| 1   | CA    | 298    | A    | Sidechain |
| 1   | CA    | 305    | G    | Sidechain |
| 1   | CA    | 323    | U    | Sidechain |
| 1   | CA    | 324    | G    | Sidechain |
| 1   | CA    | 352    | C    | Sidechain |
| 1   | CA    | 356    | A    | Sidechain |
| 1   | CA    | 380    | G    | Sidechain |
| 1   | CA    | 401    | C    | Sidechain |
| 1   | CA    | 432    | A    | Sidechain |
| 1   | CA    | 437    | U    | Sidechain |
| 1   | CA    | 45     | U    | Sidechain |
| 1   | CA    | 454    | C    | Sidechain |
| 1   | CA    | 47     | C    | Sidechain |
| 1   | CA    | 498    | U    | Sidechain |
| 1   | CA    | 5      | U    | Sidechain |
| 1   | CA    | 526    | C    | Sidechain |
| 1   | CA    | 530    | G    | Sidechain |
| 1   | CA    | 551    | U    | Sidechain |
| 1   | CA    | 560    | U    | Sidechain |
| 1   | CA    | 576    | G    | Sidechain |
| 1   | CA    | 62     | U    | Sidechain |
| 1   | CA    | 657    | G    | Sidechain |
| 1   | CA    | 690    | G    | Sidechain |
| 1   | CA    | 691    | G    | Sidechain |
| 1   | CA    | 723    | U    | Sidechain |
| 1   | CA    | 730    | G    | Sidechain |
| 1   | CA    | 754    | C    | Sidechain |
| 1   | CA    | 789    | U    | Sidechain |
| 1   | CA    | 835    | U    | Sidechain |
| 1   | CA    | 838    | G    | Sidechain |

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| Mol | Chain | Res     | Type | Group     |
|-----|-------|---------|------|-----------|
| 1   | CA    | 870     | U    | Sidechain |
| 1   | CA    | 879     | C    | Sidechain |
| 1   | CA    | 898     | G    | Sidechain |
| 1   | CA    | 901     | A    | Sidechain |
| 1   | CA    | 920     | U    | Sidechain |
| 1   | CA    | 922     | G    | Sidechain |
| 1   | CA    | 935     | A    | Sidechain |
| 1   | CA    | 952     | U    | Sidechain |
| 1   | CA    | 966     | G    | Sidechain |
| 1   | CA    | 974     | A    | Sidechain |
| 1   | CA    | 994     | A    | Sidechain |
| 1   | CA    | 995     | C    | Sidechain |
| 13  | CM    | 70      | LEU  | Mainchain |
| 22  | CV    | 10      | U    | Sidechain |
| 22  | CV    | 6       | G    | Sidechain |
| 23  | CW    | 35      | G    | Sidechain |
| 23  | CW    | 71      | A    | Sidechain |
| 54  | D5    | 52      | TYR  | Sidechain |
| 55  | D6    | 46      | HIS  | Sidechain |
| 27  | DA    | 1034    | G    | Sidechain |
| 27  | DA    | 1142(A) | A    | Sidechain |
| 27  | DA    | 1165    | U    | Sidechain |
| 27  | DA    | 1171    | G    | Sidechain |
| 27  | DA    | 1188    | U    | Sidechain |
| 27  | DA    | 1190    | G    | Sidechain |
| 27  | DA    | 120     | U    | Sidechain |
| 27  | DA    | 1248    | G    | Sidechain |
| 27  | DA    | 125     | G    | Sidechain |
| 27  | DA    | 1282    | U    | Sidechain |
| 27  | DA    | 1289    | C    | Sidechain |
| 27  | DA    | 1298    | C    | Sidechain |
| 27  | DA    | 1300    | U    | Sidechain |
| 27  | DA    | 1309    | G    | Sidechain |
| 27  | DA    | 1311    | G    | Sidechain |
| 27  | DA    | 1332    | G    | Sidechain |
| 27  | DA    | 135     | G    | Sidechain |
| 27  | DA    | 1373    | A    | Sidechain |
| 27  | DA    | 1379    | A    | Sidechain |
| 27  | DA    | 1396    | U    | Sidechain |
| 27  | DA    | 145     | G    | Sidechain |
| 27  | DA    | 1461    | G    | Sidechain |
| 27  | DA    | 1494    | A    | Sidechain |

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| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 27  | DA    | 15     | G    | Sidechain |
| 27  | DA    | 151    | C    | Sidechain |
| 27  | DA    | 154(A) | C    | Sidechain |
| 27  | DA    | 1558   | A    | Sidechain |
| 27  | DA    | 1567   | A    | Sidechain |
| 27  | DA    | 157    | U    | Sidechain |
| 27  | DA    | 1633   | G    | Sidechain |
| 27  | DA    | 1648   | C    | Sidechain |
| 27  | DA    | 1664   | A    | Sidechain |
| 27  | DA    | 1702   | G    | Sidechain |
| 27  | DA    | 1769   | G    | Sidechain |
| 27  | DA    | 1772   | G    | Sidechain |
| 27  | DA    | 1780   | A    | Sidechain |
| 27  | DA    | 1781   | C    | Sidechain |
| 27  | DA    | 1782   | C    | Sidechain |
| 27  | DA    | 1783   | A    | Sidechain |
| 27  | DA    | 1801   | G    | Sidechain |
| 27  | DA    | 1815   | A    | Sidechain |
| 27  | DA    | 1816   | G    | Sidechain |
| 27  | DA    | 1841   | U    | Sidechain |
| 27  | DA    | 1849   | G    | Sidechain |
| 27  | DA    | 185    | U    | Sidechain |
| 27  | DA    | 1854   | A    | Sidechain |
| 27  | DA    | 1926   | U    | Sidechain |
| 27  | DA    | 1963   | U    | Sidechain |
| 27  | DA    | 197    | A    | Sidechain |
| 27  | DA    | 1980   | G    | Sidechain |
| 27  | DA    | 1990   | C    | Sidechain |
| 27  | DA    | 1992   | G    | Sidechain |
| 27  | DA    | 1993   | U    | Sidechain |
| 27  | DA    | 200    | U    | Sidechain |
| 27  | DA    | 2009   | G    | Sidechain |
| 27  | DA    | 2019   | A    | Sidechain |
| 27  | DA    | 2023   | G    | Sidechain |
| 27  | DA    | 2034   | U    | Sidechain |
| 27  | DA    | 2036   | C    | Sidechain |
| 27  | DA    | 2052   | G    | Sidechain |
| 27  | DA    | 2068   | U    | Sidechain |
| 27  | DA    | 2096   | U    | Sidechain |
| 27  | DA    | 2113   | U    | Sidechain |
| 27  | DA    | 2127   | G    | Sidechain |
| 27  | DA    | 2134   | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 27  | DA    | 2222 | G    | Sidechain |
| 27  | DA    | 223  | A    | Sidechain |
| 27  | DA    | 2244 | U    | Sidechain |
| 27  | DA    | 2248 | C    | Sidechain |
| 27  | DA    | 2251 | G    | Sidechain |
| 27  | DA    | 227  | A    | Sidechain |
| 27  | DA    | 2278 | A    | Sidechain |
| 27  | DA    | 229  | A    | Sidechain |
| 27  | DA    | 2305 | A    | Sidechain |
| 27  | DA    | 2335 | A    | Sidechain |
| 27  | DA    | 2347 | C    | Sidechain |
| 27  | DA    | 2348 | U    | Sidechain |
| 27  | DA    | 2381 | C    | Sidechain |
| 27  | DA    | 2387 | U    | Sidechain |
| 27  | DA    | 2401 | U    | Sidechain |
| 27  | DA    | 2419 | U    | Sidechain |
| 27  | DA    | 2424 | C    | Sidechain |
| 27  | DA    | 2428 | G    | Sidechain |
| 27  | DA    | 2431 | U    | Sidechain |
| 27  | DA    | 2466 | C    | Sidechain |
| 27  | DA    | 248  | G    | Sidechain |
| 27  | DA    | 249  | C    | Sidechain |
| 27  | DA    | 2498 | C    | Sidechain |
| 27  | DA    | 2500 | U    | Sidechain |
| 27  | DA    | 2504 | U    | Sidechain |
| 27  | DA    | 2524 | G    | Sidechain |
| 27  | DA    | 2525 | G    | Sidechain |
| 27  | DA    | 2569 | G    | Sidechain |
| 27  | DA    | 2572 | A    | Sidechain |
| 27  | DA    | 2578 | G    | Sidechain |
| 27  | DA    | 2593 | U    | Sidechain |
| 27  | DA    | 2596 | U    | Sidechain |
| 27  | DA    | 2597 | G    | Sidechain |
| 27  | DA    | 2599 | G    | Sidechain |
| 27  | DA    | 2611 | U    | Sidechain |
| 27  | DA    | 2612 | C    | Sidechain |
| 27  | DA    | 2613 | U    | Sidechain |
| 27  | DA    | 2622 | C    | Sidechain |
| 27  | DA    | 2637 | U    | Sidechain |
| 27  | DA    | 2647 | U    | Sidechain |
| 27  | DA    | 2654 | A    | Sidechain |
| 27  | DA    | 2656 | U    | Sidechain |

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| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 27  | DA    | 2681   | C    | Sidechain |
| 27  | DA    | 2702   | U    | Sidechain |
| 27  | DA    | 272    | G    | Sidechain |
| 27  | DA    | 272(B) | G    | Sidechain |
| 27  | DA    | 2732   | G    | Sidechain |
| 27  | DA    | 2805   | G    | Sidechain |
| 27  | DA    | 2834   | G    | Sidechain |
| 27  | DA    | 284    | U    | Sidechain |
| 27  | DA    | 295    | G    | Sidechain |
| 27  | DA    | 303    | U    | Sidechain |
| 27  | DA    | 308    | G    | Sidechain |
| 27  | DA    | 313    | C    | Sidechain |
| 27  | DA    | 329    | G    | Sidechain |
| 27  | DA    | 334    | C    | Sidechain |
| 27  | DA    | 346    | A    | Sidechain |
| 27  | DA    | 372    | G    | Sidechain |
| 27  | DA    | 384    | U    | Sidechain |
| 27  | DA    | 400    | G    | Sidechain |
| 27  | DA    | 403    | U    | Sidechain |
| 27  | DA    | 405    | U    | Sidechain |
| 27  | DA    | 411    | G    | Sidechain |
| 27  | DA    | 451    | C    | Sidechain |
| 27  | DA    | 458    | G    | Sidechain |
| 27  | DA    | 467    | G    | Sidechain |
| 27  | DA    | 474    | G    | Sidechain |
| 27  | DA    | 476    | G    | Sidechain |
| 27  | DA    | 489    | G    | Sidechain |
| 27  | DA    | 497    | A    | Sidechain |
| 27  | DA    | 504    | U    | Sidechain |
| 27  | DA    | 524    | U    | Sidechain |
| 27  | DA    | 530    | G    | Sidechain |
| 27  | DA    | 567    | A    | Sidechain |
| 27  | DA    | 588    | U    | Sidechain |
| 27  | DA    | 593    | G    | Sidechain |
| 27  | DA    | 594    | U    | Sidechain |
| 27  | DA    | 597    | U    | Sidechain |
| 27  | DA    | 61     | G    | Sidechain |
| 27  | DA    | 634    | C    | Sidechain |
| 27  | DA    | 671    | C    | Sidechain |
| 27  | DA    | 673    | C    | Sidechain |
| 27  | DA    | 675    | A    | Sidechain |
| 27  | DA    | 695    | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 27  | DA    | 73  | A    | Sidechain |
| 27  | DA    | 734 | A    | Sidechain |
| 27  | DA    | 742 | G    | Sidechain |
| 27  | DA    | 784 | A    | Sidechain |
| 27  | DA    | 79  | G    | Sidechain |
| 27  | DA    | 793 | A    | Sidechain |
| 27  | DA    | 859 | G    | Sidechain |
| 27  | DA    | 860 | U    | Sidechain |
| 27  | DA    | 89  | G    | Sidechain |
| 27  | DA    | 919 | G    | Sidechain |
| 27  | DA    | 950 | G    | Sidechain |
| 27  | DA    | 976 | C    | Sidechain |
| 27  | DA    | 979 | G    | Sidechain |
| 27  | DA    | 986 | C    | Sidechain |
| 27  | DA    | 989 | G    | Sidechain |
| 28  | DB    | 116 | G    | Sidechain |
| 28  | DB    | 117 | G    | Sidechain |
| 28  | DB    | 13  | A    | Sidechain |
| 28  | DB    | 34  | U    | Sidechain |
| 28  | DB    | 35  | U    | Sidechain |
| 28  | DB    | 66  | A    | Sidechain |
| 30  | DD    | 62  | TYR  | Sidechain |
| 36  | DN    | 4   | TYR  | Sidechain |

## 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    | 32141 | 0        | 16225    | 1913    | 0            |
| 1   | CA    | 32141 | 0        | 16225    | 2200    | 0            |
| 2   | AB    | 1901  | 0        | 1951     | 267     | 0            |
| 2   | CB    | 1901  | 0        | 1951     | 267     | 0            |
| 3   | AC    | 1613  | 0        | 1677     | 233     | 0            |
| 3   | CC    | 1613  | 0        | 1677     | 215     | 0            |
| 4   | AD    | 1703  | 0        | 1764     | 222     | 0            |
| 4   | CD    | 1703  | 0        | 1764     | 256     | 0            |
| 5   | AE    | 1147  | 0        | 1207     | 175     | 0            |
| 5   | CE    | 1147  | 0        | 1207     | 184     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | AF    | 843   | 0        | 857      | 110     | 0            |
| 6   | CF    | 843   | 0        | 857      | 121     | 0            |
| 7   | AG    | 1257  | 0        | 1296     | 180     | 0            |
| 7   | CG    | 1257  | 0        | 1296     | 149     | 0            |
| 8   | AH    | 1116  | 0        | 1177     | 206     | 0            |
| 8   | CH    | 1116  | 0        | 1177     | 178     | 0            |
| 9   | AI    | 1005  | 0        | 1032     | 145     | 0            |
| 9   | CI    | 1006  | 0        | 1034     | 145     | 0            |
| 10  | AJ    | 795   | 0        | 840      | 164     | 0            |
| 10  | CJ    | 795   | 0        | 840      | 157     | 0            |
| 11  | AK    | 885   | 0        | 904      | 123     | 0            |
| 11  | CK    | 885   | 0        | 904      | 113     | 0            |
| 12  | AL    | 971   | 0        | 1057     | 167     | 0            |
| 12  | CL    | 971   | 0        | 1057     | 185     | 0            |
| 13  | AM    | 947   | 0        | 999      | 196     | 0            |
| 13  | CM    | 910   | 0        | 931      | 185     | 0            |
| 14  | AN    | 492   | 0        | 533      | 99      | 0            |
| 14  | CN    | 492   | 0        | 533      | 106     | 0            |
| 15  | AO    | 734   | 0        | 771      | 116     | 0            |
| 15  | CO    | 734   | 0        | 771      | 104     | 0            |
| 16  | AP    | 701   | 0        | 720      | 113     | 0            |
| 16  | CP    | 701   | 0        | 720      | 96      | 0            |
| 17  | AQ    | 824   | 0        | 891      | 109     | 0            |
| 17  | CQ    | 824   | 0        | 891      | 121     | 0            |
| 18  | AR    | 574   | 0        | 644      | 90      | 0            |
| 18  | CR    | 574   | 0        | 644      | 73      | 0            |
| 19  | AS    | 630   | 0        | 652      | 109     | 0            |
| 19  | CS    | 630   | 0        | 652      | 106     | 0            |
| 20  | AT    | 763   | 0        | 861      | 118     | 0            |
| 20  | CT    | 763   | 0        | 861      | 132     | 0            |
| 21  | AU    | 209   | 0        | 221      | 24      | 0            |
| 21  | CU    | 209   | 0        | 221      | 33      | 0            |
| 22  | AV    | 213   | 0        | 110      | 6       | 0            |
| 22  | CV    | 213   | 0        | 110      | 12      | 0            |
| 23  | AW    | 1593  | 0        | 810      | 80      | 0            |
| 23  | CW    | 1593  | 0        | 810      | 75      | 0            |
| 24  | AX    | 1640  | 0        | 837      | 69      | 0            |
| 24  | CX    | 1640  | 0        | 837      | 73      | 0            |
| 25  | AY    | 1591  | 0        | 810      | 83      | 0            |
| 25  | CY    | 1591  | 0        | 810      | 87      | 0            |
| 26  | AZ    | 48    | 0        | 40       | 12      | 0            |
| 26  | CZ    | 48    | 0        | 40       | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27  | BA    | 60311 | 0        | 30410    | 3523    | 0            |
| 27  | DA    | 60313 | 0        | 30409    | 3995    | 0            |
| 28  | BB    | 2528  | 0        | 1285     | 121     | 0            |
| 28  | DB    | 2528  | 0        | 1285     | 141     | 0            |
| 29  | BC    | 1142  | 0        | 865      | 101     | 0            |
| 29  | DC    | 1142  | 0        | 865      | 133     | 0            |
| 30  | BD    | 2105  | 0        | 2182     | 414     | 0            |
| 30  | DD    | 2105  | 0        | 2182     | 386     | 0            |
| 31  | BE    | 1564  | 0        | 1629     | 294     | 0            |
| 31  | DE    | 1564  | 0        | 1629     | 325     | 0            |
| 32  | BF    | 1624  | 0        | 1677     | 321     | 0            |
| 32  | DF    | 1624  | 0        | 1677     | 262     | 0            |
| 33  | BG    | 1474  | 0        | 1535     | 226     | 0            |
| 33  | DG    | 1474  | 0        | 1535     | 259     | 0            |
| 34  | BH    | 1252  | 0        | 1316     | 235     | 0            |
| 34  | DH    | 1223  | 0        | 1282     | 194     | 0            |
| 35  | BI    | 1042  | 0        | 1031     | 193     | 0            |
| 35  | DI    | 1046  | 0        | 1035     | 152     | 0            |
| 36  | BN    | 1105  | 0        | 1180     | 171     | 0            |
| 36  | DN    | 1105  | 0        | 1180     | 214     | 0            |
| 37  | BO    | 933   | 0        | 996      | 170     | 0            |
| 37  | DO    | 933   | 0        | 996      | 165     | 0            |
| 38  | BP    | 1114  | 0        | 1187     | 295     | 0            |
| 38  | DP    | 1114  | 0        | 1187     | 327     | 0            |
| 39  | BQ    | 1122  | 0        | 1179     | 176     | 0            |
| 39  | DQ    | 1107  | 0        | 1166     | 203     | 0            |
| 40  | BR    | 960   | 0        | 1021     | 164     | 0            |
| 40  | DR    | 960   | 0        | 1021     | 179     | 0            |
| 41  | BS    | 771   | 0        | 832      | 160     | 0            |
| 41  | DS    | 777   | 0        | 825      | 148     | 0            |
| 42  | BT    | 1142  | 0        | 1202     | 279     | 0            |
| 42  | DT    | 1142  | 0        | 1202     | 273     | 0            |
| 43  | BU    | 958   | 0        | 1015     | 185     | 0            |
| 43  | DU    | 958   | 0        | 1015     | 196     | 0            |
| 44  | BV    | 779   | 0        | 852      | 166     | 0            |
| 44  | DV    | 779   | 0        | 852      | 168     | 0            |
| 45  | BW    | 896   | 0        | 953      | 103     | 0            |
| 45  | DW    | 896   | 0        | 953      | 157     | 0            |
| 46  | BX    | 726   | 0        | 778      | 103     | 0            |
| 46  | DX    | 726   | 0        | 778      | 127     | 0            |
| 47  | BY    | 776   | 0        | 870      | 215     | 0            |
| 47  | DY    | 776   | 0        | 870      | 191     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48  | BZ    | 1404  | 0        | 1432     | 184     | 0            |
| 48  | DZ    | 1404  | 0        | 1432     | 221     | 0            |
| 49  | B0    | 662   | 0        | 688      | 89      | 0            |
| 49  | D0    | 662   | 0        | 688      | 103     | 0            |
| 50  | B1    | 715   | 0        | 766      | 118     | 0            |
| 50  | D1    | 732   | 0        | 808      | 98      | 0            |
| 51  | B2    | 598   | 0        | 653      | 112     | 0            |
| 51  | D2    | 598   | 0        | 653      | 84      | 0            |
| 52  | B3    | 468   | 0        | 523      | 56      | 0            |
| 52  | D3    | 468   | 0        | 523      | 84      | 0            |
| 53  | B4    | 226   | 0        | 226      | 40      | 0            |
| 53  | D4    | 226   | 0        | 227      | 33      | 0            |
| 54  | B5    | 459   | 0        | 476      | 76      | 0            |
| 54  | D5    | 459   | 0        | 476      | 70      | 0            |
| 55  | B6    | 411   | 0        | 403      | 122     | 0            |
| 55  | D6    | 390   | 0        | 403      | 103     | 0            |
| 56  | B7    | 419   | 0        | 467      | 49      | 0            |
| 56  | D7    | 419   | 0        | 467      | 80      | 0            |
| 57  | B8    | 508   | 0        | 576      | 122     | 0            |
| 57  | D8    | 508   | 0        | 576      | 135     | 0            |
| 58  | B9    | 299   | 0        | 323      | 50      | 0            |
| 58  | D9    | 299   | 0        | 323      | 49      | 0            |
| 59  | AA    | 133   | 0        | 0        | 0       | 0            |
| 59  | AC    | 1     | 0        | 0        | 0       | 0            |
| 59  | AD    | 1     | 0        | 0        | 0       | 0            |
| 59  | AE    | 1     | 0        | 0        | 0       | 0            |
| 59  | AF    | 1     | 0        | 0        | 0       | 0            |
| 59  | AH    | 1     | 0        | 0        | 0       | 0            |
| 59  | AK    | 2     | 0        | 0        | 0       | 0            |
| 59  | AL    | 1     | 0        | 0        | 0       | 0            |
| 59  | AO    | 1     | 0        | 0        | 0       | 0            |
| 59  | AT    | 2     | 0        | 0        | 0       | 0            |
| 59  | AW    | 7     | 0        | 0        | 0       | 0            |
| 59  | AX    | 7     | 0        | 0        | 0       | 0            |
| 59  | AY    | 2     | 0        | 0        | 0       | 0            |
| 59  | B0    | 2     | 0        | 0        | 0       | 0            |
| 59  | B5    | 1     | 0        | 0        | 0       | 0            |
| 59  | BA    | 400   | 0        | 0        | 0       | 0            |
| 59  | BB    | 1     | 0        | 0        | 0       | 0            |
| 59  | BD    | 1     | 0        | 0        | 0       | 0            |
| 59  | BE    | 1     | 0        | 0        | 0       | 0            |
| 59  | BF    | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 59  | BH    | 1      | 0        | 0        | 0       | 0            |
| 59  | BN    | 1      | 0        | 0        | 0       | 0            |
| 59  | BP    | 1      | 0        | 0        | 0       | 0            |
| 59  | BQ    | 1      | 0        | 0        | 0       | 0            |
| 59  | BR    | 1      | 0        | 0        | 0       | 0            |
| 59  | BU    | 1      | 0        | 0        | 0       | 0            |
| 59  | BX    | 1      | 0        | 0        | 0       | 0            |
| 59  | BY    | 1      | 0        | 0        | 1       | 0            |
| 59  | BZ    | 1      | 0        | 0        | 0       | 0            |
| 59  | CA    | 92     | 0        | 0        | 0       | 0            |
| 59  | CE    | 2      | 0        | 0        | 0       | 0            |
| 59  | CQ    | 1      | 0        | 0        | 0       | 0            |
| 59  | CV    | 2      | 0        | 0        | 0       | 0            |
| 59  | CX    | 3      | 0        | 0        | 0       | 0            |
| 59  | D5    | 2      | 0        | 0        | 0       | 0            |
| 59  | D6    | 1      | 0        | 0        | 0       | 0            |
| 59  | DA    | 275    | 0        | 0        | 0       | 0            |
| 59  | DB    | 1      | 0        | 0        | 0       | 0            |
| 59  | DD    | 3      | 0        | 0        | 0       | 0            |
| 59  | DE    | 3      | 0        | 0        | 0       | 0            |
| 59  | DF    | 1      | 0        | 0        | 0       | 0            |
| 59  | DR    | 1      | 0        | 0        | 0       | 0            |
| 59  | DZ    | 1      | 0        | 0        | 0       | 0            |
| 60  | AD    | 1      | 0        | 0        | 1       | 0            |
| 60  | B4    | 1      | 0        | 0        | 0       | 0            |
| 60  | B5    | 1      | 0        | 0        | 0       | 0            |
| 60  | B9    | 1      | 0        | 0        | 0       | 0            |
| 60  | CD    | 1      | 0        | 0        | 1       | 0            |
| 60  | D4    | 1      | 0        | 0        | 0       | 0            |
| 60  | D5    | 1      | 0        | 0        | 0       | 0            |
| 60  | D9    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 294559 | 0        | 198754   | 25938   | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

All (25938) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BP:59:LEU:HA   | 38:BP:61:ARG:CZ   | 1.58                     | 1.32              |
| 30:DD:231:HIS:ND1 | 30:DD:232:PRO:HD2 | 1.55                     | 1.20              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:CA:1363(A):A:H1' | 1:CA:1365:G:N7      | 1.57                     | 1.19              |
| 40:BR:100:LEU:HD21 | 40:BR:113:LEU:HD13  | 1.24                     | 1.19              |
| 27:BA:2787:C:H1'   | 31:BE:61:ARG:HG3    | 1.25                     | 1.18              |
| 2:CB:91:PRO:HG3    | 2:CB:154:LEU:HB2    | 1.24                     | 1.17              |
| 32:BF:3:GLU:HB2    | 32:BF:19:GLU:HB2    | 1.23                     | 1.16              |
| 41:BS:97:ARG:NH2   | 41:BS:98:VAL:HA     | 1.60                     | 1.16              |
| 27:BA:2680:C:H5'   | 31:BE:189:PRO:HA    | 1.28                     | 1.16              |
| 47:BY:96:ILE:HB    | 47:BY:99:CYS:HB2    | 1.21                     | 1.15              |
| 12:AL:29:PHE:HB3   | 12:AL:81:LEU:HD11   | 1.19                     | 1.15              |
| 34:BH:85:LYS:HD3   | 34:BH:133:VAL:HB    | 1.24                     | 1.15              |
| 37:BO:14:THR:HG21  | 37:BO:86:ILE:HD12   | 1.21                     | 1.15              |
| 12:AL:44:LYS:HB3   | 12:AL:45:PRO:HD3    | 1.15                     | 1.15              |
| 36:DN:70:LYS:HG2   | 36:DN:87:LEU:HD12   | 1.25                     | 1.15              |
| 46:BX:30:VAL:HG21  | 46:BX:39:ILE:HD11   | 1.26                     | 1.15              |
| 27:DA:242:G:H5''   | 57:D8:62:LEU:HD13   | 1.29                     | 1.14              |
| 12:CL:44:LYS:HB3   | 12:CL:45:PRO:HD2    | 1.23                     | 1.14              |
| 38:DP:45:LEU:HD23  | 38:DP:46:LYS:H      | 0.97                     | 1.14              |
| 38:BP:65:ARG:NH2   | 57:B8:15:LYS:HB2    | 1.60                     | 1.14              |
| 39:DQ:12:GLN:HE21  | 39:DQ:72:LYS:HG3    | 1.11                     | 1.13              |
| 1:CA:1101:A:H4'    | 1:CA:1102:A:O5'     | 1.46                     | 1.13              |
| 27:DA:271(S):G:H2' | 27:DA:271(T):C:H5'' | 1.26                     | 1.13              |
| 5:AE:50:GLU:HG3    | 5:AE:52:PRO:HD2     | 1.14                     | 1.13              |
| 30:BD:165:ILE:HD13 | 30:BD:175:LEU:HD21  | 1.24                     | 1.13              |
| 30:DD:239:ARG:HG2  | 30:DD:239:ARG:HH21  | 1.11                     | 1.13              |
| 27:BA:27:G:N2      | 27:BA:512:G:H2'     | 1.63                     | 1.13              |
| 48:DZ:149:LEU:HD23 | 48:DZ:170:ILE:HG13  | 1.30                     | 1.13              |
| 11:AK:127:LYS:HE2  | 11:AK:127:LYS:HA    | 1.24                     | 1.12              |
| 48:DZ:157:PRO:HG2  | 48:DZ:160:VAL:HG21  | 1.30                     | 1.12              |
| 4:CD:9:CYS:SG      | 4:CD:22:LYS:HD2     | 1.88                     | 1.12              |
| 33:BG:106:LEU:O    | 33:BG:111:LEU:HB2   | 1.48                     | 1.12              |
| 27:BA:661:C:H4'    | 38:BP:16:ARG:HH12   | 1.02                     | 1.12              |
| 12:CL:43:LYS:HG2   | 12:CL:44:LYS:H      | 1.12                     | 1.12              |
| 13:CM:25:ILE:HD11  | 13:CM:66:LEU:HD23   | 1.28                     | 1.12              |
| 27:BA:480:A:H1'    | 47:BY:44:ILE:HG21   | 1.31                     | 1.11              |
| 42:DT:65:LYS:HZ2   | 42:DT:66:VAL:N      | 1.47                     | 1.11              |
| 27:BA:2729:G:H1'   | 31:BE:187:ALA:HB2   | 1.31                     | 1.11              |
| 32:BF:2:LYS:H      | 32:BF:2:LYS:HD3     | 1.08                     | 1.11              |
| 31:BE:59:VAL:HG22  | 31:BE:60:ASN:H      | 1.11                     | 1.11              |
| 54:B5:4:HIS:HB3    | 54:B5:5:PRO:HD3     | 1.23                     | 1.11              |
| 2:CB:172:ILE:HD12  | 2:CB:172:ILE:H      | 1.06                     | 1.11              |
| 1:CA:1347:G:N2     | 1:CA:1373:G:H2'     | 1.66                     | 1.11              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:BF:67:GLN:HG3   | 32:BF:67:GLN:O     | 1.48                     | 1.10              |
| 2:CB:204:ASN:HD21  | 2:CB:207:ALA:HB3   | 1.15                     | 1.10              |
| 5:AE:129:ILE:HG22  | 5:AE:130:ASN:H     | 1.16                     | 1.10              |
| 44:BV:18:LEU:HD13  | 44:BV:19:LYS:H     | 1.14                     | 1.10              |
| 16:CP:82:GLN:HE21  | 16:CP:82:GLN:N     | 1.49                     | 1.10              |
| 1:CA:721:G:H4'     | 1:CA:722:A:O5'     | 1.52                     | 1.10              |
| 38:DP:71:VAL:HG13  | 38:DP:72:PRO:HD3   | 1.17                     | 1.10              |
| 42:DT:65:LYS:NZ    | 42:DT:66:VAL:H     | 1.50                     | 1.10              |
| 27:DA:1891:G:H2'   | 27:DA:1892:C:H6    | 1.11                     | 1.10              |
| 42:BT:79:HIS:O     | 42:BT:81:PRO:HD3   | 1.50                     | 1.10              |
| 5:AE:33:VAL:HG23   | 5:AE:43:LEU:HD13   | 1.35                     | 1.09              |
| 17:AQ:17:LYS:HG2   | 17:AQ:47:PRO:HA    | 1.13                     | 1.09              |
| 27:BA:2327:A:H2'   | 27:BA:2328:A:C8    | 1.87                     | 1.09              |
| 29:BC:83:ILE:HG23  | 29:BC:94:VAL:HG23  | 1.34                     | 1.09              |
| 27:DA:1891:G:H2'   | 27:DA:1892:C:C6    | 1.87                     | 1.09              |
| 31:DE:144:ARG:HH11 | 31:DE:144:ARG:HG3  | 1.11                     | 1.09              |
| 32:DF:7:TYR:HB3    | 32:DF:16:GLY:H     | 1.15                     | 1.09              |
| 8:AH:63:LEU:HB3    | 8:AH:65:TYR:HE1    | 1.13                     | 1.09              |
| 44:BV:19:LYS:HG2   | 44:BV:94:LEU:HB2   | 1.26                     | 1.09              |
| 27:BA:285:C:H2'    | 27:BA:286:C:H5''   | 1.21                     | 1.09              |
| 19:CS:19:VAL:HG11  | 19:CS:44:MET:HG3   | 1.27                     | 1.09              |
| 27:DA:2230:G:H1'   | 50:D1:45:ASN:HB2   | 1.23                     | 1.09              |
| 1:AA:1080:A:H5'    | 5:AE:14:ARG:HH21   | 1.03                     | 1.09              |
| 27:BA:2476:A:H2'   | 27:BA:2477:C:H5''  | 1.34                     | 1.09              |
| 34:BH:85:LYS:HZ2   | 34:BH:133:VAL:HG11 | 1.16                     | 1.09              |
| 42:BT:27:THR:O     | 42:BT:28:VAL:HG23  | 1.50                     | 1.09              |
| 12:CL:44:LYS:HB3   | 12:CL:45:PRO:CD    | 1.83                     | 1.09              |
| 27:DA:1796:U:H2'   | 27:DA:1797:C:H6    | 1.14                     | 1.09              |
| 43:DU:55:ARG:HA    | 43:DU:58:ARG:HB2   | 1.31                     | 1.09              |
| 27:BA:2701:C:H3'   | 27:BA:2702:U:H5''  | 1.16                     | 1.08              |
| 42:BT:91:ARG:HB3   | 42:BT:116:ALA:HA   | 1.32                     | 1.08              |
| 14:CN:37:PHE:HB3   | 14:CN:39:LEU:HG    | 1.32                     | 1.08              |
| 27:DA:492:A:H2'    | 27:DA:493:G:O4'    | 1.51                     | 1.08              |
| 47:DY:75:ILE:HG13  | 47:DY:79:CYS:HA    | 1.29                     | 1.08              |
| 29:BC:41:VAL:HA    | 29:BC:213:TYR:HA   | 1.26                     | 1.08              |
| 47:BY:46:LYS:HB2   | 47:BY:62:GLU:HG2   | 1.28                     | 1.08              |
| 27:DA:35:G:H1'     | 27:DA:454:A:H1'    | 1.30                     | 1.08              |
| 41:BS:34:HIS:NE2   | 41:BS:54:LEU:HB2   | 1.69                     | 1.08              |
| 1:CA:1250:A:H4'    | 9:CI:68:GLY:H      | 1.16                     | 1.08              |
| 30:DD:118:VAL:HG22 | 30:DD:119:ALA:H    | 1.06                     | 1.08              |
| 27:DA:1568:G:H5''  | 30:DD:61:LEU:HD23  | 1.31                     | 1.08              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:BD:24:ILE:HG13   | 30:BD:25:THR:N     | 1.66                     | 1.08              |
| 37:BO:104:ARG:HH12  | 42:BT:35:LYS:HE2   | 1.16                     | 1.08              |
| 4:CD:82:ALA:HB1     | 4:CD:89:THR:HG23   | 1.34                     | 1.08              |
| 12:CL:52:VAL:HG22   | 12:CL:66:TYR:HA    | 1.34                     | 1.08              |
| 27:DA:1826:G:H4'    | 30:DD:242:ARG:HH21 | 1.09                     | 1.08              |
| 52:B3:23:LEU:H      | 52:B3:23:LEU:HD12  | 1.17                     | 1.08              |
| 27:DA:94(A):G:H2'   | 27:DA:95:G:H5''    | 1.27                     | 1.08              |
| 44:BV:19:LYS:HE2    | 44:BV:20:LEU:H     | 1.14                     | 1.08              |
| 31:BE:77:ILE:HG22   | 31:BE:78:LEU:H     | 1.15                     | 1.07              |
| 1:CA:1347:G:H22     | 1:CA:1373:G:H2'    | 1.03                     | 1.07              |
| 54:B5:16:ARG:HG2    | 54:B5:16:ARG:HH11  | 1.12                     | 1.07              |
| 27:DA:1884:A:H2'    | 27:DA:1885:A:H5''  | 1.32                     | 1.07              |
| 27:DA:2833:G:H3'    | 27:DA:2834:G:H5''  | 1.11                     | 1.07              |
| 30:DD:24:ILE:HG13   | 30:DD:25:THR:H     | 1.18                     | 1.07              |
| 27:BA:1378:A:O2'    | 27:BA:1379:A:H5'   | 1.52                     | 1.07              |
| 27:BA:1899:G:N2     | 27:BA:1902:C:H41   | 1.53                     | 1.07              |
| 27:BA:2801(A):A:H4' | 27:BA:2802:G:H5'   | 1.31                     | 1.07              |
| 42:DT:42:ILE:H      | 42:DT:42:ILE:HD12  | 1.14                     | 1.07              |
| 1:AA:473:G:H2'      | 1:AA:474:G:H8      | 1.19                     | 1.07              |
| 45:DW:7:ALA:HB3     | 45:DW:103:ILE:HB   | 1.30                     | 1.07              |
| 47:DY:76:CYS:SG     | 47:DY:77:PRO:HD2   | 1.94                     | 1.07              |
| 33:BG:39:ILE:HD11   | 33:BG:155:MET:HB2  | 1.32                     | 1.07              |
| 41:DS:85:VAL:H      | 41:DS:106:ARG:HB2  | 1.14                     | 1.07              |
| 43:BU:92:ARG:HH11   | 43:BU:92:ARG:HB2   | 0.97                     | 1.07              |
| 1:CA:1363(A):A:H4'  | 1:CA:1364:U:H5''   | 1.36                     | 1.07              |
| 1:CA:979:C:H3'      | 1:CA:980:C:H5''    | 1.36                     | 1.07              |
| 11:AK:32:ILE:HD12   | 11:AK:72:ALA:HB2   | 1.31                     | 1.07              |
| 27:BA:1884:A:H2'    | 27:BA:1885:A:H5''  | 1.37                     | 1.07              |
| 27:DA:906:G:H2'     | 27:DA:907:U:H5''   | 1.32                     | 1.07              |
| 38:DP:45:LEU:HD23   | 38:DP:46:LYS:N     | 1.69                     | 1.07              |
| 27:BA:1747(A):G:H2' | 27:BA:1748:G:H5''  | 1.23                     | 1.07              |
| 27:DA:2701:C:H3'    | 27:DA:2702:U:C5'   | 1.84                     | 1.07              |
| 31:DE:77:ILE:HG22   | 31:DE:78:LEU:H     | 0.94                     | 1.07              |
| 17:AQ:18:THR:HG23   | 17:AQ:69:LYS:HE3   | 1.37                     | 1.06              |
| 7:CG:113:GLU:HB2    | 7:CG:119:ARG:HG2   | 1.31                     | 1.06              |
| 11:CK:32:ILE:HD11   | 11:CK:41:THR:HG22  | 1.20                     | 1.06              |
| 55:D6:33:LYS:HA     | 55:D6:33:LYS:HE2   | 1.32                     | 1.06              |
| 33:DG:22:ARG:HH11   | 33:DG:22:ARG:HB3   | 1.18                     | 1.06              |
| 4:AD:196:LEU:HD12   | 4:AD:196:LEU:H     | 1.14                     | 1.06              |
| 47:BY:15:VAL:HG22   | 47:BY:72:VAL:HG12  | 1.37                     | 1.06              |
| 56:D7:41:ARG:NH1    | 56:D7:41:ARG:HB2   | 1.71                     | 1.06              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DP:63:PRO:HB3   | 57:D8:13:ARG:HB3   | 1.20                     | 1.06              |
| 1:AA:1080:A:H5'    | 5:AE:14:ARG:NH2    | 1.69                     | 1.06              |
| 27:BA:2317:C:C2'   | 27:BA:2318:G:H5'   | 1.85                     | 1.06              |
| 36:DN:34:LEU:HD11  | 36:DN:120:LEU:HD23 | 1.37                     | 1.06              |
| 47:DY:27:VAL:HA    | 47:DY:28:LYS:HZ1   | 1.20                     | 1.06              |
| 20:AT:71:THR:HG22  | 20:AT:72:LEU:H     | 1.16                     | 1.06              |
| 27:BA:1020:A:H4'   | 27:BA:1021:A:O5'   | 1.56                     | 1.06              |
| 14:CN:41:ARG:HG3   | 14:CN:42:ILE:H     | 1.19                     | 1.06              |
| 27:DA:586:A:H5'    | 32:DF:89:VAL:HG21  | 1.38                     | 1.06              |
| 23:AW:30:A:H2'     | 23:AW:31:U:H5''    | 1.38                     | 1.06              |
| 27:BA:2701:C:H3'   | 27:BA:2702:U:C5'   | 1.85                     | 1.06              |
| 27:DA:704:G:H2'    | 27:DA:726:G:H22    | 1.17                     | 1.06              |
| 27:DA:2787:C:H1'   | 31:DE:61:ARG:HG3   | 1.37                     | 1.06              |
| 31:DE:36:ARG:NH2   | 31:DE:88:GLY:HA3   | 1.71                     | 1.05              |
| 30:BD:26:LYS:NZ    | 30:BD:82:ILE:H     | 1.54                     | 1.05              |
| 27:DA:2701:C:H3'   | 27:DA:2702:U:H5''  | 1.06                     | 1.05              |
| 27:BA:286:C:C2'    | 27:BA:287:C:H5'    | 1.84                     | 1.05              |
| 44:BV:41:GLY:HA3   | 44:BV:45:THR:OG1   | 1.56                     | 1.05              |
| 1:CA:1137:C:H4'    | 1:CA:1138:G:C2     | 1.91                     | 1.05              |
| 43:BU:90:VAL:HG12  | 43:BU:91:ASP:H     | 1.21                     | 1.05              |
| 2:CB:69:LEU:HD22   | 2:CB:91:PRO:HB2    | 1.30                     | 1.05              |
| 50:B1:37:ILE:HG22  | 50:B1:38:SER:H     | 1.14                     | 1.05              |
| 55:B6:40:CYS:HA    | 55:B6:46:HIS:HB3   | 1.33                     | 1.05              |
| 39:BQ:110:THR:HG23 | 39:BQ:113:GLN:HB2  | 1.37                     | 1.05              |
| 45:BW:6:ILE:HG12   | 45:BW:104:THR:HG23 | 1.37                     | 1.05              |
| 38:DP:48:PRO:HG2   | 38:DP:49:ARG:H     | 1.20                     | 1.05              |
| 47:DY:81:LYS:HD3   | 47:DY:97:ARG:HB3   | 1.36                     | 1.05              |
| 47:BY:76:CYS:SG    | 47:BY:77:PRO:HD2   | 1.97                     | 1.05              |
| 1:CA:1106:G:H5''   | 3:CC:172:ARG:HG2   | 1.39                     | 1.04              |
| 6:AF:43:LEU:H      | 6:AF:43:LEU:HD12   | 1.21                     | 1.04              |
| 55:D6:40:CYS:HA    | 55:D6:46:HIS:HB3   | 1.39                     | 1.04              |
| 27:DA:228:A:O2'    | 27:DA:229:A:H5'    | 1.55                     | 1.04              |
| 27:BA:2483:C:H3'   | 27:BA:2484:G:H5''  | 1.37                     | 1.04              |
| 18:CR:82:THR:HG22  | 18:CR:83:GLU:H     | 1.19                     | 1.04              |
| 31:DE:36:ARG:HH22  | 31:DE:88:GLY:HA3   | 1.19                     | 1.04              |
| 46:DX:35:THR:O     | 46:DX:39:ILE:HG12  | 1.55                     | 1.04              |
| 48:DZ:32:LEU:HD23  | 48:DZ:89:VAL:HG21  | 1.39                     | 1.04              |
| 4:AD:7:PRO:HB2     | 4:AD:10:ARG:HD2    | 1.32                     | 1.04              |
| 31:DE:179:GLU:HB3  | 31:DE:181:LEU:HD13 | 1.40                     | 1.04              |
| 47:DY:42:VAL:HB    | 47:DY:65:ALA:HB3   | 1.36                     | 1.04              |
| 27:BA:1685:C:H2'   | 27:BA:1686:C:H5''  | 1.39                     | 1.04              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:BD:118:VAL:HG22 | 30:BD:119:ALA:H    | 1.20                     | 1.04              |
| 34:BH:44:VAL:HG12  | 34:BH:45:VAL:H     | 1.15                     | 1.04              |
| 42:BT:89:VAL:HB    | 42:BT:91:ARG:HE    | 1.21                     | 1.04              |
| 13:CM:13:LYS:HA    | 13:CM:44:ARG:HH11  | 1.18                     | 1.04              |
| 27:DA:2579:C:O3'   | 31:DE:131:ALA:HB2  | 1.57                     | 1.04              |
| 41:DS:52:SER:HB2   | 41:DS:55:ALA:HB3   | 1.36                     | 1.04              |
| 27:BA:286:C:H2'    | 27:BA:287:C:H5'    | 1.36                     | 1.04              |
| 1:CA:198:G:H2'     | 1:CA:199:G:C8      | 1.93                     | 1.04              |
| 4:CD:173:TRP:NE1   | 4:CD:189:PRO:HG3   | 1.72                     | 1.04              |
| 44:DV:18:LEU:HD22  | 44:DV:19:LYS:H     | 1.21                     | 1.04              |
| 35:DI:133:HIS:HB2  | 35:DI:134:PRO:HD3  | 1.39                     | 1.03              |
| 47:DY:28:LYS:HB3   | 47:DY:39:VAL:H     | 1.21                     | 1.03              |
| 9:AI:53:VAL:HG23   | 9:AI:54:ASP:H      | 1.21                     | 1.03              |
| 47:BY:26:LYS:HG2   | 47:BY:27:VAL:H     | 1.23                     | 1.03              |
| 38:DP:59:LEU:HA    | 38:DP:61:ARG:CZ    | 1.87                     | 1.03              |
| 55:B6:40:CYS:HA    | 55:B6:46:HIS:CB    | 1.87                     | 1.03              |
| 51:D2:4:SER:HA     | 51:D2:7:ARG:HH11   | 1.20                     | 1.03              |
| 8:AH:34:GLU:HB3    | 8:AH:118:VAL:HG21  | 1.39                     | 1.03              |
| 30:BD:60:ARG:HD3   | 30:BD:86:PRO:HG2   | 1.39                     | 1.03              |
| 48:BZ:81:ARG:HH21  | 48:BZ:83:GLU:HA    | 1.19                     | 1.03              |
| 2:AB:69:LEU:HB3    | 2:AB:162:ILE:HG22  | 1.37                     | 1.03              |
| 12:CL:29:PHE:HB3   | 12:CL:81:LEU:HD11  | 1.37                     | 1.03              |
| 27:DA:1798:U:H5'   | 30:DD:259:THR:HG22 | 1.40                     | 1.03              |
| 27:BA:2701:C:C3'   | 27:BA:2702:U:H5''  | 1.89                     | 1.03              |
| 40:DR:61:HIS:O     | 40:DR:65:LEU:HD13  | 1.57                     | 1.03              |
| 1:AA:676:A:H1'     | 11:AK:115:PRO:HB3  | 1.38                     | 1.03              |
| 30:BD:186:HIS:CD2  | 30:BD:188:GLU:H    | 1.75                     | 1.03              |
| 1:AA:533:A:O2'     | 1:AA:534:U:H5''    | 1.58                     | 1.03              |
| 46:BX:64:LYS:NZ    | 46:BX:73:ARG:HE    | 1.56                     | 1.03              |
| 27:DA:869:G:H2'    | 27:DA:870:A:H8     | 1.19                     | 1.03              |
| 42:DT:28:VAL:HG22  | 42:DT:47:GLY:H     | 1.15                     | 1.03              |
| 1:AA:299:G:H2'     | 1:AA:300:A:C8      | 1.93                     | 1.03              |
| 1:CA:377:G:H1      | 1:CA:386:C:H42     | 1.07                     | 1.03              |
| 41:DS:24:LEU:HB3   | 41:DS:85:VAL:HG12  | 1.33                     | 1.03              |
| 2:AB:51:LEU:HD23   | 2:AB:201:ILE:HD12  | 1.35                     | 1.02              |
| 19:AS:32:LYS:HA    | 19:AS:50:ALA:HB3   | 1.39                     | 1.02              |
| 27:BA:857:C:H5'    | 49:B0:77:ARG:HH22  | 1.19                     | 1.02              |
| 27:BA:954:G:H5''   | 39:BQ:13:GLN:HG2   | 1.40                     | 1.02              |
| 46:BX:63:LYS:HE3   | 46:BX:72:LYS:HE3   | 1.38                     | 1.02              |
| 58:D9:15:LYS:HE2   | 58:D9:17:ILE:HD11  | 1.40                     | 1.02              |
| 27:DA:90:U:O2'     | 27:DA:92:A:H5''    | 1.58                     | 1.02              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:DD:133:LEU:HD11  | 30:DD:175:LEU:HD11 | 1.41                     | 1.02              |
| 33:DG:22:ARG:HB3    | 33:DG:22:ARG:NH1   | 1.74                     | 1.02              |
| 42:DT:88:ILE:HG22   | 42:DT:89:VAL:H     | 1.21                     | 1.02              |
| 16:AP:18:ARG:HH11   | 16:AP:35:LYS:HD2   | 1.24                     | 1.02              |
| 43:BU:104:GLN:HE22  | 43:BU:105:VAL:HG23 | 1.20                     | 1.02              |
| 39:DQ:16:ARG:HG2    | 39:DQ:17:LEU:H     | 1.20                     | 1.02              |
| 41:DS:30:ARG:HH22   | 41:DS:62:LYS:HD2   | 1.17                     | 1.02              |
| 3:CC:53:ALA:HB2     | 3:CC:115:LEU:HD21  | 1.41                     | 1.02              |
| 27:BA:1249:U:H5'    | 27:BA:1249:U:H6    | 1.21                     | 1.02              |
| 42:BT:28:VAL:HG22   | 42:BT:46:GLU:HA    | 1.41                     | 1.02              |
| 42:BT:89:VAL:HG12   | 42:BT:91:ARG:HG2   | 1.39                     | 1.02              |
| 12:CL:15:VAL:HG23   | 12:CL:16:ARG:H     | 1.22                     | 1.02              |
| 49:D0:41:ARG:HD2    | 49:D0:41:ARG:H     | 1.21                     | 1.02              |
| 1:AA:1305:G:H22     | 1:AA:1331:G:H2'    | 1.24                     | 1.02              |
| 31:DE:77:ILE:HG22   | 31:DE:78:LEU:N     | 1.72                     | 1.02              |
| 9:AI:53:VAL:HG23    | 9:AI:55:ALA:H      | 1.23                     | 1.02              |
| 1:CA:234:C:H2'      | 1:CA:235:C:H6      | 1.24                     | 1.01              |
| 1:CA:957:U:H2'      | 1:CA:959:A:OP2     | 1.60                     | 1.01              |
| 11:CK:32:ILE:HD12   | 11:CK:72:ALA:HB2   | 1.35                     | 1.01              |
| 43:DU:92:ARG:HG2    | 43:DU:92:ARG:HH11  | 1.22                     | 1.01              |
| 27:BA:795:C:H2'     | 27:BA:796:C:H6     | 1.25                     | 1.01              |
| 26:CZ:4:SER:O       | 26:CZ:5:UAL:N1     | 1.93                     | 1.01              |
| 27:DA:2498:C:O2'    | 27:DA:2499:C:H5''  | 1.60                     | 1.01              |
| 1:AA:376:G:H5''     | 16:AP:5:ARG:HB2    | 1.39                     | 1.01              |
| 3:AC:155:GLY:HA3    | 3:AC:163:ALA:HB1   | 1.42                     | 1.01              |
| 17:AQ:7:THR:HG22    | 17:AQ:58:GLU:HG2   | 1.43                     | 1.01              |
| 1:CA:562:C:H4'      | 1:CA:563:A:H5'     | 1.43                     | 1.01              |
| 23:CW:73:C:H2'      | 23:CW:74:C:H5'     | 1.38                     | 1.01              |
| 39:DQ:36:ALA:HB2    | 39:DQ:103:MET:SD   | 2.00                     | 1.01              |
| 1:AA:100:C:H2'      | 1:AA:101:A:C8      | 1.95                     | 1.01              |
| 19:AS:10:PHE:HZ     | 19:AS:70:LYS:HZ3   | 1.04                     | 1.01              |
| 27:BA:1747(A):G:C2' | 27:BA:1748:G:H5''  | 1.89                     | 1.01              |
| 1:CA:161:A:H2'      | 1:CA:162:A:C8      | 1.94                     | 1.01              |
| 50:D1:52:ARG:HG3    | 50:D1:53:VAL:H     | 1.21                     | 1.01              |
| 27:BA:1784:A:H4'    | 27:BA:1785:A:O5'   | 1.57                     | 1.01              |
| 31:BE:36:ARG:NH2    | 31:BE:88:GLY:HA3   | 1.75                     | 1.00              |
| 56:D7:41:ARG:HH11   | 56:D7:41:ARG:HB2   | 0.87                     | 1.00              |
| 27:DA:2833:G:H3'    | 27:DA:2834:G:C5'   | 1.90                     | 1.00              |
| 32:BF:83:PHE:O      | 32:BF:84:VAL:HB    | 1.61                     | 1.00              |
| 27:DA:2572:A:H5''   | 27:DA:2574:G:H4'   | 1.39                     | 1.00              |
| 34:BH:8:PRO:HD2     | 34:BH:69:ARG:HD2   | 1.42                     | 1.00              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 11:CK:22:HIS:HB3    | 11:CK:29:ILE:HG23 | 1.41                     | 1.00              |
| 2:AB:18:GLY:H       | 2:AB:42:ILE:HG22  | 1.23                     | 1.00              |
| 57:D8:6:THR:HG22    | 57:D8:63:PRO:HD3  | 1.37                     | 1.00              |
| 55:D6:13:CYS:O      | 55:D6:21:TYR:HA   | 1.62                     | 1.00              |
| 38:DP:9:ASN:ND2     | 38:DP:10:PRO:HD3  | 1.76                     | 1.00              |
| 1:CA:1363(A):A:H4'  | 1:CA:1364:U:C5'   | 1.91                     | 1.00              |
| 2:CB:32:ILE:HD11    | 2:CB:40:HIS:HB3   | 1.41                     | 1.00              |
| 27:DA:519:U:H2'     | 27:DA:520:G:C8    | 1.95                     | 1.00              |
| 27:BA:1879:C:H2'    | 27:BA:1880:C:H5'' | 1.43                     | 1.00              |
| 1:CA:309:G:H1'      | 1:CA:608:A:H2     | 1.27                     | 1.00              |
| 27:BA:969:U:OP1     | 52:B3:17:LYS:HD3  | 1.61                     | 1.00              |
| 30:BD:49:ILE:HD11   | 30:BD:52:ARG:HA   | 1.40                     | 1.00              |
| 41:BS:24:LEU:HB3    | 41:BS:85:VAL:HG12 | 1.42                     | 1.00              |
| 41:BS:97:ARG:HH21   | 41:BS:98:VAL:CA   | 1.74                     | 1.00              |
| 48:BZ:68:THR:HG22   | 48:BZ:89:VAL:HA   | 1.40                     | 1.00              |
| 27:BA:2331:G:H4'    | 49:B0:43:THR:H    | 1.27                     | 1.00              |
| 32:BF:123:LEU:HD12  | 32:BF:124:LEU:H   | 1.24                     | 1.00              |
| 27:DA:2838:G:H1'    | 40:DR:45:ARG:NH1  | 1.77                     | 1.00              |
| 27:BA:1273:U:H5''   | 27:BA:1273:U:H6   | 1.27                     | 0.99              |
| 27:BA:2317:C:H2'    | 27:BA:2318:G:H5'  | 1.40                     | 0.99              |
| 27:BA:2068:U:H3     | 27:BA:2430:A:H2   | 1.01                     | 0.99              |
| 33:DG:105:LYS:HE2   | 53:D4:52:SER:HB3  | 1.44                     | 0.99              |
| 27:BA:2755:C:H3'    | 58:B9:19:ARG:NH2  | 1.77                     | 0.99              |
| 45:BW:90:ARG:HB2    | 45:BW:90:ARG:HH11 | 1.27                     | 0.99              |
| 3:AC:16:ARG:NH1     | 3:AC:16:ARG:HB2   | 1.77                     | 0.99              |
| 27:BA:360:G:H2'     | 27:BA:361:G:H8    | 1.27                     | 0.99              |
| 27:BA:1173:G:H3'    | 27:BA:1174:A:H5'  | 1.44                     | 0.99              |
| 30:BD:43:ARG:HD2    | 30:BD:44:ASN:OD1  | 1.61                     | 0.99              |
| 15:CO:35:ARG:HH21   | 15:CO:59:MET:HE2  | 1.23                     | 0.99              |
| 1:AA:1101:A:H4'     | 1:AA:1102:A:O5'   | 1.62                     | 0.99              |
| 7:AG:54:THR:OG1     | 7:AG:56:GLN:HG2   | 1.60                     | 0.99              |
| 16:CP:43:LYS:HA     | 16:CP:48:TRP:HB3  | 1.43                     | 0.99              |
| 27:DA:1747(A):G:H2' | 27:DA:1748:G:H5'' | 1.40                     | 0.99              |
| 2:AB:172:ILE:HD12   | 2:AB:172:ILE:H    | 1.26                     | 0.99              |
| 46:DX:12:VAL:HG23   | 46:DX:13:LEU:H    | 1.23                     | 0.99              |
| 2:CB:96:ARG:H       | 2:CB:96:ARG:HD2   | 1.24                     | 0.99              |
| 27:DA:633:A:H2'     | 27:DA:634:C:H5'   | 1.41                     | 0.99              |
| 8:CH:60:ARG:HH11    | 8:CH:60:ARG:HG3   | 1.26                     | 0.99              |
| 36:DN:133:GLN:HG2   | 36:DN:135:PRO:HD3 | 1.44                     | 0.99              |
| 27:BA:1865:G:H5'    | 27:BA:1866:C:OP2  | 1.61                     | 0.99              |
| 1:AA:580:U:H3       | 1:AA:761:G:H1     | 1.10                     | 0.99              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:AK:124:LYS:HE3 | 11:AK:125:PHE:HE1  | 1.25                     | 0.98              |
| 52:B3:29:ARG:HB2  | 52:B3:33:GLN:HE22  | 1.26                     | 0.98              |
| 27:BA:1603:A:C8   | 27:BA:1603:A:H5'   | 1.98                     | 0.98              |
| 1:CA:992:U:H4'    | 1:CA:993:G:O5'     | 1.62                     | 0.98              |
| 27:DA:200:U:H5'   | 27:DA:200:U:H6     | 1.27                     | 0.98              |
| 32:DF:111:ALA:HB2 | 32:DF:206:ILE:HG21 | 1.43                     | 0.98              |
| 1:AA:452:A:HO2'   | 1:AA:453:A:H8      | 1.02                     | 0.98              |
| 30:BD:33:LEU:O    | 30:BD:34:VAL:HG12  | 1.63                     | 0.98              |
| 27:DA:2732:G:H3'  | 27:DA:2733:A:H5'   | 1.40                     | 0.98              |
| 27:BA:1184:G:OP1  | 52:B3:29:ARG:HD3   | 1.63                     | 0.98              |
| 1:CA:198:G:H2'    | 1:CA:199:G:H8      | 1.23                     | 0.98              |
| 36:BN:63:THR:HG22 | 36:BN:64:GLY:H     | 1.28                     | 0.98              |
| 1:CA:1003:G:H2'   | 1:CA:1004:A:H4'    | 1.41                     | 0.98              |
| 1:CA:1321:C:H5''  | 1:CA:1322:C:H5''   | 1.45                     | 0.98              |
| 20:CT:50:GLU:HA   | 20:CT:100:ILE:HG12 | 1.46                     | 0.98              |
| 30:DD:242:ARG:H   | 30:DD:242:ARG:HD2  | 1.25                     | 0.98              |
| 4:AD:25:ARG:HH12  | 4:AD:30:LYS:HG3    | 1.25                     | 0.98              |
| 45:BW:88:ARG:HB2  | 45:BW:92:ARG:HB2   | 1.45                     | 0.98              |
| 12:CL:52:VAL:HG13 | 12:CL:65:ALA:O     | 1.63                     | 0.98              |
| 1:AA:751:U:H4'    | 15:AO:24:SER:HA    | 1.44                     | 0.98              |
| 32:BF:66:PRO:HD2  | 32:BF:70:THR:HG21  | 1.44                     | 0.98              |
| 47:DY:28:LYS:HB2  | 47:DY:38:ILE:H     | 1.24                     | 0.98              |
| 16:AP:82:GLN:HE21 | 16:AP:83:GLU:H     | 1.04                     | 0.98              |
| 27:BA:1336:A:H2'  | 27:BA:1337:G:H8    | 1.28                     | 0.98              |
| 27:DA:514:A:O2'   | 27:DA:515:A:H5'    | 1.63                     | 0.98              |
| 41:BS:68:GLN:HA   | 41:BS:71:ARG:HD2   | 1.42                     | 0.97              |
| 20:CT:26:ASN:HB2  | 20:CT:71:THR:HG23  | 1.42                     | 0.97              |
| 23:CW:42:G:H3'    | 23:CW:43:C:H5''    | 1.46                     | 0.97              |
| 6:AF:62:TRP:CH2   | 6:AF:64:GLN:HB2    | 1.99                     | 0.97              |
| 30:BD:60:ARG:HD3  | 30:BD:86:PRO:CG    | 1.95                     | 0.97              |
| 12:CL:76:GLU:O    | 12:CL:77:HIS:HB2   | 1.62                     | 0.97              |
| 55:D6:32:ASN:HD22 | 55:D6:33:LYS:N     | 1.63                     | 0.97              |
| 55:D6:39:TYR:O    | 55:D6:46:HIS:HB2   | 1.64                     | 0.97              |
| 31:DE:26:ILE:HG22 | 31:DE:27:LEU:H     | 1.24                     | 0.97              |
| 41:DS:19:LYS:O    | 41:DS:20:ARG:HD3   | 1.62                     | 0.97              |
| 42:DT:51:ARG:HD2  | 42:DT:62:THR:HG23  | 1.46                     | 0.97              |
| 48:DZ:150:HIS:HB3 | 48:DZ:169:THR:HG22 | 1.41                     | 0.97              |
| 27:BA:2467:C:H4'  | 39:BQ:123:HIS:CD2  | 1.98                     | 0.97              |
| 41:BS:46:VAL:HG12 | 41:BS:47:THR:H     | 1.25                     | 0.97              |
| 27:DA:2172:U:H1'  | 27:DA:2173:A:OP1   | 1.63                     | 0.97              |
| 1:AA:721:G:H4'    | 1:AA:722:A:O5'     | 1.63                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:1775:U:H2'  | 27:DA:1776:G:H5'  | 1.45                     | 0.97              |
| 1:AA:1321:C:H5'   | 1:AA:1322:C:H5''  | 1.47                     | 0.97              |
| 34:BH:156:ALA:C   | 34:BH:158:HIS:H   | 1.52                     | 0.97              |
| 27:BA:285:C:C2'   | 27:BA:286:C:H5''  | 1.93                     | 0.97              |
| 35:DI:93:THR:HG22 | 35:DI:119:PRO:HB3 | 1.47                     | 0.97              |
| 27:BA:740:U:H6    | 27:BA:740:U:H5'   | 1.26                     | 0.97              |
| 1:CA:1066:C:H5''  | 1:CA:1066:C:C6    | 1.99                     | 0.97              |
| 56:D7:41:ARG:HH11 | 56:D7:41:ARG:CB   | 1.76                     | 0.97              |
| 27:DA:1410:G:H2'  | 27:DA:1411:C:C6   | 1.99                     | 0.97              |
| 30:DD:24:ILE:HG13 | 30:DD:25:THR:N    | 1.79                     | 0.97              |
| 8:AH:60:ARG:HG3   | 8:AH:60:ARG:HH11  | 1.27                     | 0.97              |
| 10:AJ:49:VAL:HG23 | 14:AN:41:ARG:HD2  | 1.43                     | 0.97              |
| 37:BO:22:ILE:HG12 | 37:BO:41:ALA:HA   | 1.47                     | 0.97              |
| 38:BP:23:PRO:O    | 38:BP:33:ARG:HD2  | 1.62                     | 0.97              |
| 47:BY:27:VAL:HA   | 47:BY:28:LYS:NZ   | 1.80                     | 0.97              |
| 43:DU:90:VAL:HG12 | 43:DU:91:ASP:H    | 1.29                     | 0.97              |
| 44:DV:2:PHE:HB2   | 44:DV:42:GLY:HA2  | 1.47                     | 0.97              |
| 30:BD:31:LYS:HE3  | 30:BD:33:LEU:HD22 | 1.47                     | 0.97              |
| 1:CA:189(L):G:H2' | 1:CA:190:U:C6     | 1.99                     | 0.97              |
| 11:AK:124:LYS:HE3 | 11:AK:125:PHE:CE1 | 1.99                     | 0.96              |
| 13:AM:37:THR:HG21 | 13:AM:56:LEU:HA   | 1.46                     | 0.96              |
| 32:BF:89:VAL:HG12 | 32:BF:90:PHE:H    | 1.27                     | 0.96              |
| 9:CI:82:ALA:HB1   | 9:CI:96:LEU:HD11  | 1.46                     | 0.96              |
| 55:B6:15:GLU:OE2  | 55:B6:18:ARG:NE   | 1.97                     | 0.96              |
| 27:BA:2784:C:H1'  | 31:BE:42:ASP:OD1  | 1.64                     | 0.96              |
| 47:BY:7:VAL:HB    | 47:BY:8:LYS:HZ2   | 1.30                     | 0.96              |
| 1:CA:179:A:H2'    | 1:CA:180:U:H6     | 1.26                     | 0.96              |
| 27:DA:71:A:H5''   | 27:DA:73:A:C8     | 2.00                     | 0.96              |
| 12:AL:44:LYS:HB3  | 12:AL:45:PRO:CD   | 1.95                     | 0.96              |
| 20:AT:26:ASN:HD22 | 20:AT:26:ASN:H    | 0.99                     | 0.96              |
| 27:BA:2792:G:O2'  | 27:BA:2793:G:H8   | 1.48                     | 0.96              |
| 31:BE:59:VAL:HG22 | 31:BE:60:ASN:N    | 1.80                     | 0.96              |
| 43:DU:92:ARG:HD2  | 44:DV:11:GLN:NE2  | 1.80                     | 0.96              |
| 20:AT:26:ASN:O    | 20:AT:30:LYS:HB2  | 1.66                     | 0.96              |
| 40:BR:79:LEU:HA   | 40:BR:83:ILE:HG13 | 1.45                     | 0.96              |
| 27:DA:571:A:H4'   | 27:DA:572:A:OP1   | 1.63                     | 0.96              |
| 27:BA:1899:G:H22  | 27:BA:1902:C:N4   | 1.64                     | 0.96              |
| 27:BA:661:C:H4'   | 38:BP:16:ARG:NH1  | 1.79                     | 0.96              |
| 44:BV:19:LYS:CE   | 44:BV:20:LEU:H    | 1.78                     | 0.96              |
| 47:BY:96:ILE:CB   | 47:BY:99:CYS:HB2  | 1.94                     | 0.96              |
| 55:D6:40:CYS:CA   | 55:D6:46:HIS:HB3  | 1.95                     | 0.96              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 27:DA:35:G:C1'     | 27:DA:454:A:H1'     | 1.95                     | 0.96              |
| 30:DD:44:ASN:HB2   | 30:DD:49:ILE:HA     | 1.47                     | 0.96              |
| 46:BX:9:LEU:HA     | 51:B2:36:ARG:HH21   | 1.29                     | 0.96              |
| 27:BA:2200:C:H5''  | 27:BA:2200:C:H6     | 1.29                     | 0.96              |
| 44:BV:5:VAL:HG11   | 44:BV:57:VAL:HG11   | 1.47                     | 0.96              |
| 1:CA:1163:C:H2'    | 1:CA:1164:G:C8      | 2.01                     | 0.96              |
| 9:CI:9:ARG:HG3     | 9:CI:14:VAL:HG22    | 1.48                     | 0.96              |
| 27:DA:2712:U:HO2'  | 27:DA:2712(A):A:H8  | 0.98                     | 0.96              |
| 4:AD:17:VAL:HG11   | 4:AD:197:PRO:HG3    | 1.45                     | 0.96              |
| 17:AQ:43:LEU:HD12  | 17:AQ:68:ARG:HG2    | 1.48                     | 0.96              |
| 27:BA:1562:A:H2'   | 27:BA:1563:G:C8     | 2.00                     | 0.96              |
| 38:DP:13:ASN:C     | 38:DP:13:ASN:HD22   | 1.69                     | 0.96              |
| 1:CA:373:A:H2'     | 1:CA:374:A:H8       | 1.30                     | 0.96              |
| 1:CA:309:G:H1'     | 1:CA:608:A:C2       | 2.00                     | 0.96              |
| 4:CD:153:ARG:HB3   | 4:CD:153:ARG:HH11   | 1.30                     | 0.96              |
| 27:DA:2555:U:H2'   | 27:DA:2556:C:H5'    | 1.46                     | 0.96              |
| 44:BV:46:VAL:HG22  | 44:BV:47:VAL:H      | 1.30                     | 0.95              |
| 3:CC:47:LEU:HD11   | 3:CC:76:VAL:HG12    | 1.44                     | 0.95              |
| 27:DA:2758:A:H2'   | 27:DA:2759:G:H5''   | 1.48                     | 0.95              |
| 50:B1:25:LYS:HA    | 50:B1:29:GLY:HA2    | 1.48                     | 0.95              |
| 27:BA:2206:G:H21   | 27:BA:2207:G:H5'    | 1.30                     | 0.95              |
| 9:CI:125:TYR:HE2   | 9:CI:127:LYS:HB2    | 1.31                     | 0.95              |
| 50:D1:51:VAL:HG21  | 50:D1:74:VAL:HG21   | 1.46                     | 0.95              |
| 27:BA:1434:A:H61   | 27:BA:1558:A:N6     | 1.63                     | 0.95              |
| 43:BU:92:ARG:HE    | 44:BV:11:GLN:HB2    | 1.31                     | 0.95              |
| 27:DA:2475:C:H42   | 27:DA:2529:G:H22    | 0.99                     | 0.95              |
| 27:DA:373:U:H2'    | 27:DA:374:A:H8      | 1.29                     | 0.95              |
| 27:DA:2749:A:H4'   | 34:DH:62:LYS:HB3    | 1.47                     | 0.95              |
| 37:BO:93:PRO:HG3   | 37:BO:114:ILE:CD1   | 1.96                     | 0.95              |
| 27:DA:49:A:H61     | 27:DA:177:G:H2'     | 1.32                     | 0.95              |
| 32:DF:155:LEU:HD23 | 32:DF:192:LEU:HD21  | 1.49                     | 0.95              |
| 1:AA:911:U:H2'     | 1:AA:912:C:C6       | 2.01                     | 0.95              |
| 12:AL:73:ASN:HD22  | 12:AL:74:LEU:H      | 0.96                     | 0.95              |
| 27:DA:271(S):G:C2' | 27:DA:271(T):C:H5'' | 1.96                     | 0.95              |
| 51:D2:13:ALA:HA    | 51:D2:16:LEU:HD12   | 1.48                     | 0.95              |
| 27:DA:13:A:H1'     | 27:DA:15:G:N7       | 1.82                     | 0.95              |
| 1:AA:1422:G:H1     | 1:AA:1478:C:H42     | 1.15                     | 0.95              |
| 1:AA:553:A:H2'     | 1:AA:554:C:C6       | 2.02                     | 0.95              |
| 28:BB:40:U:H3      | 28:BB:43:C:H5''     | 1.31                     | 0.95              |
| 47:BY:31:LEU:HB2   | 47:BY:32:PRO:HA     | 1.45                     | 0.95              |
| 1:CA:386:C:H2'     | 1:CA:387:U:H5'      | 1.49                     | 0.95              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:DO:71:ARG:HB3  | 37:DO:72:PRO:HD2   | 1.48                     | 0.95              |
| 11:AK:32:ILE:HD11 | 11:AK:41:THR:HB    | 1.49                     | 0.95              |
| 27:BA:2832:U:H4'  | 27:BA:2833:G:H5''  | 1.46                     | 0.95              |
| 20:CT:72:LEU:HD23 | 20:CT:73:HIS:H     | 1.29                     | 0.95              |
| 27:DA:2107:C:H42  | 27:DA:2182:G:H1    | 1.13                     | 0.95              |
| 27:BA:1798:U:H5'  | 30:BD:259:THR:HG22 | 1.49                     | 0.95              |
| 6:CF:38:GLU:O     | 6:CF:39:LYS:HB2    | 1.67                     | 0.95              |
| 38:DP:39:LYS:HA   | 38:DP:39:LYS:HE2   | 1.48                     | 0.95              |
| 18:AR:53:ARG:NH2  | 18:AR:60:ALA:H     | 1.63                     | 0.95              |
| 47:BY:10:GLY:HA2  | 47:BY:27:VAL:HG13  | 1.48                     | 0.95              |
| 47:BY:27:VAL:HA   | 47:BY:28:LYS:HZ2   | 1.31                     | 0.95              |
| 1:CA:676:A:H1'    | 11:CK:115:PRO:HB3  | 1.49                     | 0.95              |
| 27:DA:52:A:O2'    | 27:DA:53:A:H8      | 1.49                     | 0.95              |
| 27:DA:543:C:H42   | 27:DA:551:G:H1     | 1.07                     | 0.95              |
| 6:AF:9:VAL:HB     | 6:AF:87:ARG:HB2    | 1.46                     | 0.94              |
| 8:AH:97:VAL:HG13  | 8:AH:98:LYS:H      | 1.30                     | 0.94              |
| 10:AJ:4:ILE:HB    | 10:AJ:74:ILE:HD11  | 1.49                     | 0.94              |
| 42:BT:50:ILE:HG13 | 42:BT:102:ILE:HD11 | 1.47                     | 0.94              |
| 5:CE:50:GLU:HB3   | 5:CE:53:LEU:HD13   | 1.49                     | 0.94              |
| 36:DN:73:THR:HG22 | 36:DN:82:LEU:HD11  | 1.49                     | 0.94              |
| 27:BA:2271:G:H4'  | 49:B0:20:ARG:NH1   | 1.82                     | 0.94              |
| 15:CO:87:ILE:HG22 | 15:CO:88:ARG:H     | 1.30                     | 0.94              |
| 27:DA:1020:A:H4'  | 27:DA:1021:A:O5'   | 1.63                     | 0.94              |
| 1:AA:707:C:O2'    | 1:AA:708:C:H5'     | 1.67                     | 0.94              |
| 38:BP:16:ARG:CZ   | 38:BP:18:ARG:HG2   | 1.97                     | 0.94              |
| 1:CA:1352:C:H2'   | 1:CA:1353:G:C8     | 2.02                     | 0.94              |
| 34:DH:12:PRO:HG2  | 34:DH:49:VAL:HA    | 1.46                     | 0.94              |
| 36:DN:4:TYR:HB2   | 43:DU:64:ARG:HH12  | 1.30                     | 0.94              |
| 27:DA:94(A):G:C2' | 27:DA:95:G:H5''    | 1.97                     | 0.94              |
| 27:BA:2263:C:H2'  | 27:BA:2264:C:H6    | 1.32                     | 0.94              |
| 32:BF:135:LYS:HB3 | 32:BF:138:GLU:HG3  | 1.46                     | 0.94              |
| 38:BP:23:PRO:HD2  | 38:BP:33:ARG:NE    | 1.81                     | 0.94              |
| 6:CF:33:TYR:HD2   | 6:CF:71:ARG:HD2    | 1.33                     | 0.94              |
| 12:AL:38:ARG:HG2  | 12:AL:39:THR:H     | 1.32                     | 0.94              |
| 54:B5:16:ARG:HH11 | 54:B5:16:ARG:CG    | 1.80                     | 0.94              |
| 55:B6:20:ASN:HD22 | 55:B6:21:TYR:H     | 1.14                     | 0.94              |
| 27:BA:554:U:O2'   | 27:BA:555:U:H5'    | 1.66                     | 0.94              |
| 27:BA:2580:U:H5'  | 31:BE:131:ALA:CB   | 1.98                     | 0.94              |
| 1:CA:1181:G:H2'   | 1:CA:1182:G:C4     | 2.01                     | 0.94              |
| 27:DA:1798:U:C5'  | 30:DD:259:THR:HG22 | 1.98                     | 0.94              |
| 1:AA:1348:U:H2'   | 1:AA:1349:A:C8     | 2.03                     | 0.94              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1348:U:H2'    | 1:AA:1349:A:H8    | 1.33                     | 0.94              |
| 4:AD:80:GLU:O      | 4:AD:84:LYS:HG2   | 1.67                     | 0.94              |
| 27:BA:1484:G:H3'   | 27:BA:1485:G:H5'' | 1.47                     | 0.94              |
| 32:BF:11:VAL:HG12  | 32:BF:12:LEU:H    | 1.32                     | 0.94              |
| 2:CB:55:PHE:HA     | 2:CB:58:ILE:HG12  | 1.47                     | 0.94              |
| 14:CN:12:ARG:C     | 14:CN:14:PRO:HD2  | 1.87                     | 0.94              |
| 1:CA:192:U:C4'     | 20:CT:103:GLY:HA2 | 1.98                     | 0.94              |
| 27:DA:154(A):C:H41 | 27:DA:172:C:H42   | 0.97                     | 0.94              |
| 27:BA:1685:C:C2'   | 27:BA:1686:C:H5'' | 1.97                     | 0.94              |
| 1:CA:1208:C:H2'    | 1:CA:1209:C:H6    | 1.32                     | 0.94              |
| 43:BU:90:VAL:HG21  | 44:BV:47:VAL:HG21 | 1.49                     | 0.94              |
| 47:BY:46:LYS:HB2   | 47:BY:62:GLU:CG   | 1.97                     | 0.94              |
| 27:DA:2870:C:H2'   | 27:DA:2871:C:H5'  | 1.48                     | 0.94              |
| 27:DA:2875:C:H4'   | 42:DT:5:ALA:HB2   | 1.49                     | 0.94              |
| 52:B3:11:SER:OG    | 52:B3:13:ILE:HD12 | 1.66                     | 0.94              |
| 41:BS:85:VAL:H     | 41:BS:106:ARG:HB2 | 1.31                     | 0.94              |
| 41:BS:82:ILE:HD13  | 41:BS:82:ILE:H    | 1.30                     | 0.94              |
| 27:DA:740:U:H6     | 27:DA:740:U:H5'   | 1.28                     | 0.94              |
| 27:BA:2836:U:H2'   | 27:BA:2837:G:C8   | 2.02                     | 0.93              |
| 30:BD:108:PRO:HG3  | 30:BD:143:HIS:NE2 | 1.83                     | 0.93              |
| 1:CA:693:G:O2'     | 7:CG:82:GLY:HA3   | 1.67                     | 0.93              |
| 13:CM:4:ILE:HG22   | 13:CM:5:ALA:H     | 1.32                     | 0.93              |
| 30:DD:43:ARG:HH11  | 30:DD:44:ASN:ND2  | 1.66                     | 0.93              |
| 39:DQ:45:GLN:H     | 39:DQ:45:GLN:HE21 | 1.05                     | 0.93              |
| 48:DZ:127:VAL:HG22 | 48:DZ:128:SER:H   | 1.32                     | 0.93              |
| 1:AA:166:G:H2'     | 1:AA:167:G:C8     | 2.02                     | 0.93              |
| 27:BA:2841:C:H2'   | 27:BA:2842:G:H8   | 1.31                     | 0.93              |
| 46:BX:64:LYS:HZ3   | 46:BX:73:ARG:HE   | 1.02                     | 0.93              |
| 8:CH:10:LEU:HD23   | 8:CH:83:ILE:HG12  | 1.51                     | 0.93              |
| 47:DY:10:GLY:HA2   | 47:DY:27:VAL:HG13 | 1.50                     | 0.93              |
| 1:AA:553:A:H2'     | 1:AA:554:C:H6     | 1.33                     | 0.93              |
| 8:AH:63:LEU:HB3    | 8:AH:65:TYR:CE1   | 2.03                     | 0.93              |
| 41:BS:102:ALA:HB3  | 41:BS:103:GLU:OE1 | 1.67                     | 0.93              |
| 46:DX:65:ARG:HD3   | 46:DX:70:LEU:HD12 | 1.48                     | 0.93              |
| 42:BT:88:ILE:HG22  | 42:BT:89:VAL:H    | 1.31                     | 0.93              |
| 43:BU:92:ARG:NH1   | 43:BU:92:ARG:HB2  | 1.83                     | 0.93              |
| 16:CP:82:GLN:HE21  | 16:CP:82:GLN:H    | 1.12                     | 0.93              |
| 27:DA:133:C:N4     | 27:DA:146:G:H1    | 1.65                     | 0.93              |
| 27:DA:34:C:O2'     | 27:DA:35:G:H5'    | 1.69                     | 0.93              |
| 28:DB:87:G:H3'     | 28:DB:88:C:H5''   | 1.50                     | 0.93              |
| 37:DO:105:GLU:HA   | 37:DO:108:GLU:HG3 | 1.51                     | 0.93              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:112:VAL:HG23  | 2:AB:149:LEU:HD13  | 1.46                     | 0.93              |
| 1:AA:1057:G:H4'    | 3:AC:196:LEU:O     | 1.68                     | 0.93              |
| 32:BF:176:LEU:HD11 | 32:BF:180:GLY:HA3  | 1.50                     | 0.93              |
| 34:BH:158:HIS:O    | 34:BH:159:GLU:HB2  | 1.69                     | 0.93              |
| 27:BA:2875:C:H4'   | 42:BT:5:ALA:HB2    | 1.51                     | 0.93              |
| 4:CD:173:TRP:HE3   | 4:CD:173:TRP:H     | 1.16                     | 0.93              |
| 20:CT:50:GLU:CA    | 20:CT:100:ILE:HG12 | 1.98                     | 0.93              |
| 30:DD:44:ASN:CB    | 30:DD:49:ILE:HA    | 1.99                     | 0.93              |
| 40:DR:38:VAL:HB    | 40:DR:39:PRO:HD3   | 1.49                     | 0.93              |
| 5:AE:43:LEU:HD22   | 5:AE:109:ILE:HD11  | 1.48                     | 0.93              |
| 25:AY:68:C:H2'     | 25:AY:69:C:H5''    | 1.51                     | 0.93              |
| 56:B7:8:ASN:HD22   | 56:B7:8:ASN:C      | 1.69                     | 0.93              |
| 38:BP:106:LEU:HD13 | 38:BP:112:LEU:HD23 | 1.51                     | 0.93              |
| 47:BY:90:LEU:HD12  | 47:BY:91:GLU:H     | 1.31                     | 0.93              |
| 27:DA:1565:C:O2'   | 27:DA:1566:A:H2'   | 1.67                     | 0.93              |
| 32:DF:16:GLY:O     | 32:DF:17:ARG:HG3   | 1.66                     | 0.93              |
| 32:DF:34:TRP:CZ2   | 38:DP:12:ALA:HB2   | 2.02                     | 0.93              |
| 35:DI:37:VAL:HG12  | 35:DI:38:LEU:HD12  | 1.48                     | 0.93              |
| 43:DU:49:HIS:HA    | 43:DU:52:ARG:HB2   | 1.51                     | 0.93              |
| 48:DZ:4:LEU:HD21   | 48:DZ:42:GLU:HB3   | 1.49                     | 0.93              |
| 27:BA:1292:U:H2'   | 27:BA:1293:C:C6    | 2.04                     | 0.93              |
| 27:BA:2172:U:H1'   | 27:BA:2173:A:OP1   | 1.69                     | 0.93              |
| 1:CA:652:U:O2'     | 1:CA:653:A:H5''    | 1.68                     | 0.93              |
| 1:CA:1320:C:O2     | 19:CS:72:GLY:HA3   | 1.68                     | 0.93              |
| 49:D0:53:MET:HB3   | 49:D0:59:LEU:HD23  | 1.51                     | 0.93              |
| 1:AA:911:U:H2'     | 1:AA:912:C:H6      | 1.33                     | 0.93              |
| 30:BD:43:ARG:NH1   | 30:BD:44:ASN:HD21  | 1.65                     | 0.93              |
| 1:CA:165:C:H2'     | 1:CA:166:G:C8      | 2.04                     | 0.93              |
| 24:CX:17:C:H2'     | 24:CX:17(B):U:H6   | 1.32                     | 0.93              |
| 27:DA:1494:A:O2'   | 27:DA:1495:A:H5''  | 1.67                     | 0.93              |
| 27:DA:2126:A:H5''  | 29:DC:36:LYS:HE2   | 1.50                     | 0.93              |
| 27:DA:881:G:H1     | 27:DA:895:U:H3     | 1.16                     | 0.93              |
| 36:DN:128:HIS:HB2  | 36:DN:130:HIS:CE1  | 2.03                     | 0.93              |
| 1:AA:438:G:H4'     | 1:AA:439:A:OP1     | 1.69                     | 0.93              |
| 30:BD:95:LEU:O     | 30:BD:95:LEU:HD12  | 1.69                     | 0.93              |
| 32:BF:89:VAL:O     | 32:BF:91:GLY:N     | 2.02                     | 0.93              |
| 34:BH:156:ALA:C    | 34:BH:158:HIS:N    | 2.22                     | 0.93              |
| 27:DA:2810:A:O2'   | 31:DE:61:ARG:HB2   | 1.69                     | 0.93              |
| 35:DI:107:VAL:HG12 | 35:DI:108:THR:H    | 1.33                     | 0.93              |
| 36:DN:15:LEU:HD12  | 36:DN:136:GLU:HG2  | 1.51                     | 0.93              |
| 58:B9:29:ASN:HD22  | 58:B9:29:ASN:H     | 0.98                     | 0.93              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:7:G:H2'      | 27:BA:8:A:C8       | 2.04                     | 0.93              |
| 38:BP:146:VAL:HG22 | 38:BP:147:LEU:H    | 1.32                     | 0.93              |
| 41:BS:52:SER:OG    | 41:BS:55:ALA:HB3   | 1.69                     | 0.93              |
| 1:CA:1502:A:H2     | 1:CA:1505:G:H1     | 0.94                     | 0.93              |
| 4:CD:200:GLU:HG2   | 4:CD:201:GLN:N     | 1.83                     | 0.93              |
| 1:AA:975:A:H4'     | 1:AA:976:G:H5''    | 1.51                     | 0.92              |
| 27:BA:152:G:H1     | 27:BA:174:C:H42    | 0.92                     | 0.92              |
| 27:BA:242:G:H5''   | 57:B8:62:LEU:HD13  | 1.49                     | 0.92              |
| 2:CB:158:LEU:HD12  | 2:CB:158:LEU:H     | 1.34                     | 0.92              |
| 27:DA:1199:U:H2'   | 27:DA:1200:C:H6    | 1.32                     | 0.92              |
| 27:DA:288:C:H42    | 27:DA:353:G:H1     | 1.07                     | 0.92              |
| 27:DA:906:G:C2'    | 27:DA:907:U:H5''   | 1.97                     | 0.92              |
| 31:DE:36:ARG:HH22  | 31:DE:88:GLY:CA    | 1.83                     | 0.92              |
| 27:DA:2476:A:N3    | 27:DA:2477:C:H5''  | 1.85                     | 0.92              |
| 27:DA:2701:C:C3'   | 27:DA:2702:U:H5''  | 1.98                     | 0.92              |
| 1:AA:15:G:H4'      | 5:AE:24:ARG:HH12   | 1.33                     | 0.92              |
| 23:AW:6:U:H3'      | 23:AW:7:A:H5''     | 1.50                     | 0.92              |
| 49:B0:23:VAL:HA    | 49:B0:38:VAL:HG22  | 1.51                     | 0.92              |
| 1:CA:1003:G:H2'    | 1:CA:1004:A:C4'    | 1.99                     | 0.92              |
| 1:CA:67:C:H2'      | 1:CA:68:G:C8       | 2.05                     | 0.92              |
| 2:CB:185:ILE:HG23  | 2:CB:199:TYR:HB2   | 1.48                     | 0.92              |
| 32:DF:125:LEU:HB3  | 32:DF:196:LEU:HD21 | 1.48                     | 0.92              |
| 39:DQ:85:LYS:HG3   | 49:D0:7:LEU:HD13   | 1.49                     | 0.92              |
| 12:AL:73:ASN:HD22  | 12:AL:74:LEU:N     | 1.67                     | 0.92              |
| 27:BA:1431:U:H2'   | 27:BA:1432:C:H6    | 1.34                     | 0.92              |
| 27:BA:27:G:H22     | 27:BA:512:G:H2'    | 1.22                     | 0.92              |
| 47:BY:87:LYS:O     | 47:BY:88:LYS:HB2   | 1.67                     | 0.92              |
| 27:DA:2223:G:H2'   | 27:DA:2224:G:H5'   | 1.49                     | 0.92              |
| 27:DA:271(N):U:H4' | 27:DA:271(O):C:OP2 | 1.69                     | 0.92              |
| 27:BA:2563:U:O2    | 27:BA:2565:A:H8    | 1.49                     | 0.92              |
| 33:BG:51:ARG:CZ    | 33:BG:53:LEU:HD21  | 1.99                     | 0.92              |
| 35:BI:111:PRO:HA   | 35:BI:114:LEU:HD21 | 1.50                     | 0.92              |
| 48:BZ:157:PRO:HG2  | 48:BZ:160:VAL:HG21 | 1.52                     | 0.92              |
| 56:D7:8:ASN:ND2    | 56:D7:11:LYS:H     | 1.66                     | 0.92              |
| 29:DC:41:VAL:HG23  | 29:DC:178:ALA:HB3  | 1.50                     | 0.92              |
| 36:DN:60:ILE:HD13  | 36:DN:99:LEU:HD23  | 1.51                     | 0.92              |
| 27:DA:1614:A:H62   | 45:DW:93:ALA:HB2   | 1.35                     | 0.92              |
| 37:BO:104:ARG:NH1  | 42:BT:35:LYS:HE2   | 1.82                     | 0.92              |
| 27:BA:2012:G:O3'   | 45:BW:96:ILE:HD11  | 1.68                     | 0.92              |
| 1:AA:490:G:H2'     | 1:AA:491:G:H8      | 1.32                     | 0.92              |
| 55:B6:36:LEU:O     | 55:B6:37:ARG:HD2   | 1.68                     | 0.92              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1899:G:H22   | 27:BA:1902:C:H41   | 0.95                     | 0.92              |
| 27:BA:571:A:H4'    | 27:BA:572:A:OP1    | 1.66                     | 0.92              |
| 38:BP:112:LEU:H    | 38:BP:128:HIS:HD2  | 1.16                     | 0.92              |
| 17:CQ:57:VAL:HG12  | 17:CQ:76:LEU:HA    | 1.48                     | 0.92              |
| 27:DA:1034:G:H5'   | 58:D9:18:ARG:HD2   | 1.51                     | 0.92              |
| 32:DF:32:LEU:HD13  | 32:DF:112:MET:HE1  | 1.51                     | 0.92              |
| 57:B8:33:ASN:ND2   | 57:B8:33:ASN:H     | 1.68                     | 0.92              |
| 32:BF:2:LYS:HE2    | 32:BF:25:PRO:HB3   | 1.50                     | 0.92              |
| 41:BS:36:TYR:HD2   | 41:BS:52:SER:HB2   | 1.34                     | 0.92              |
| 48:BZ:149:LEU:HD23 | 48:BZ:170:ILE:HG13 | 1.49                     | 0.92              |
| 57:D8:14:VAL:HG21  | 57:D8:22:VAL:HG13  | 1.50                     | 0.92              |
| 41:DS:89:ARG:HB3   | 41:DS:92:TYR:CB    | 1.98                     | 0.92              |
| 43:DU:83:LEU:HG    | 43:DU:88:ILE:HD11  | 1.49                     | 0.92              |
| 2:AB:42:ILE:HD11   | 2:AB:202:PRO:HB2   | 1.50                     | 0.92              |
| 52:B3:44:ARG:O     | 52:B3:48:GLU:HG2   | 1.69                     | 0.92              |
| 27:BA:1210:A:H5'   | 27:BA:1212:G:H5'   | 1.51                     | 0.92              |
| 27:BA:33:U:H4'     | 27:BA:34:C:OP1     | 1.70                     | 0.92              |
| 33:BG:60:LEU:HD22  | 33:BG:63:ILE:HD11  | 1.49                     | 0.92              |
| 43:BU:92:ARG:HH11  | 43:BU:92:ARG:CB    | 1.82                     | 0.92              |
| 47:BY:88:LYS:HZ3   | 47:BY:93:GLY:HA3   | 1.31                     | 0.92              |
| 27:DA:1267:U:O2'   | 27:DA:1268:A:H8    | 1.52                     | 0.92              |
| 40:DR:4:LEU:HD21   | 40:DR:8:ARG:HH21   | 1.34                     | 0.92              |
| 45:DW:73:ALA:O     | 45:DW:106:ILE:HG12 | 1.69                     | 0.92              |
| 8:AH:17:THR:HB     | 8:AH:78:GLN:OE1    | 1.69                     | 0.92              |
| 30:BD:89:SER:HB2   | 30:BD:201:HIS:CD2  | 2.05                     | 0.92              |
| 32:BF:2:LYS:N      | 32:BF:2:LYS:HD3    | 1.85                     | 0.92              |
| 41:BS:58:LEU:HD23  | 41:BS:65:VAL:HG13  | 1.52                     | 0.92              |
| 42:BT:89:VAL:HG21  | 42:BT:91:ARG:HH21  | 1.34                     | 0.92              |
| 1:CA:1502:A:H2     | 1:CA:1505:G:N1     | 1.66                     | 0.92              |
| 27:DA:2336:A:H61   | 49:D0:43:THR:HG21  | 1.32                     | 0.92              |
| 41:DS:74:ALA:HB1   | 41:DS:103:GLU:HB2  | 1.48                     | 0.92              |
| 14:AN:26:ARG:HG3   | 14:AN:27:CYS:H     | 1.36                     | 0.91              |
| 55:B6:41:PRO:HD3   | 55:B6:46:HIS:CB    | 1.99                     | 0.91              |
| 27:BA:142:A:C8     | 27:BA:1408:C:H1'   | 2.04                     | 0.91              |
| 30:BD:241:PRO:O    | 30:BD:242:ARG:HB2  | 1.70                     | 0.91              |
| 35:BI:5:LEU:HD22   | 35:BI:13:GLY:HA2   | 1.48                     | 0.91              |
| 1:AA:1157:A:H4'    | 1:AA:1158:C:O5'    | 1.69                     | 0.91              |
| 13:AM:10:PRO:HB2   | 13:AM:18:ALA:HB1   | 1.49                     | 0.91              |
| 32:BF:132:VAL:HG13 | 32:BF:133:ASN:H    | 1.33                     | 0.91              |
| 14:AN:27:CYS:O     | 14:AN:29:ARG:N     | 2.04                     | 0.91              |
| 54:B5:16:ARG:HG3   | 54:B5:17:ASP:N     | 1.85                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:2321:G:N3   | 27:BA:2321:G:H2'  | 1.84                     | 0.91              |
| 27:BA:807:U:O2'   | 27:BA:808:G:H5'   | 1.71                     | 0.91              |
| 35:BI:115:ALA:HB3 | 35:BI:129:THR:H   | 1.34                     | 0.91              |
| 1:CA:386:C:C2'    | 1:CA:387:U:H5'    | 1.99                     | 0.91              |
| 30:DD:8:PRO:HB3   | 30:DD:14:ARG:HB2  | 1.51                     | 0.91              |
| 27:DA:956:G:H5''  | 39:DQ:77:LYS:HD2  | 1.52                     | 0.91              |
| 1:AA:1305:G:N2    | 1:AA:1331:G:H2'   | 1.84                     | 0.91              |
| 27:BA:2508:G:H1   | 27:BA:2580:U:H3   | 1.18                     | 0.91              |
| 27:DA:647:G:H21   | 27:DA:2350:C:H4'  | 1.32                     | 0.91              |
| 5:AE:141:GLN:HA   | 5:AE:143:ARG:NH2  | 1.86                     | 0.91              |
| 55:B6:29:ASN:CG   | 55:B6:30:THR:H    | 1.73                     | 0.91              |
| 27:BA:2092:U:H4'  | 27:BA:2093:G:O5'  | 1.70                     | 0.91              |
| 19:CS:41:VAL:HB   | 19:CS:44:MET:HG2  | 1.52                     | 0.91              |
| 27:DA:2070:G:H2'  | 27:DA:2071:A:H8   | 1.34                     | 0.91              |
| 30:DD:60:ARG:HG3  | 30:DD:86:PRO:HB3  | 1.51                     | 0.91              |
| 7:AG:74:GLU:HG2   | 7:AG:91:VAL:HG22  | 1.52                     | 0.91              |
| 27:BA:1022:G:H4'  | 27:BA:1023:U:O5'  | 1.71                     | 0.91              |
| 30:BD:108:PRO:HG3 | 30:BD:143:HIS:HE2 | 1.35                     | 0.91              |
| 42:BT:92:GLY:C    | 42:BT:94:ALA:H    | 1.72                     | 0.91              |
| 1:CA:797:C:OP1    | 11:CK:124:LYS:HE2 | 1.69                     | 0.91              |
| 7:CG:115:ARG:O    | 7:CG:118:VAL:HG22 | 1.70                     | 0.91              |
| 1:AA:501:C:H2'    | 1:AA:502:G:C8     | 2.04                     | 0.91              |
| 5:AE:129:ILE:HG22 | 5:AE:130:ASN:N    | 1.80                     | 0.91              |
| 27:BA:2790:A:H2   | 27:BA:2791:C:H3'  | 1.36                     | 0.91              |
| 30:BD:26:LYS:HZ3  | 30:BD:82:ILE:H    | 1.09                     | 0.91              |
| 27:DA:97:C:H4'    | 51:D2:2:LYS:HB3   | 1.53                     | 0.91              |
| 38:DP:9:ASN:HD22  | 38:DP:10:PRO:HD3  | 1.35                     | 0.91              |
| 37:BO:16:ALA:HB2  | 37:BO:52:VAL:HG11 | 1.52                     | 0.91              |
| 27:DA:1762:A:H8   | 27:DA:1762:A:O5'  | 1.54                     | 0.91              |
| 2:AB:63:MET:HB3   | 2:AB:225:ALA:HB1  | 1.53                     | 0.91              |
| 27:BA:2883:A:H5'  | 27:BA:2884:U:H5'  | 1.52                     | 0.91              |
| 27:DA:1826:G:H4'  | 30:DD:242:ARG:NH2 | 1.85                     | 0.91              |
| 27:DA:333:G:H2'   | 27:DA:334:C:H6    | 1.35                     | 0.91              |
| 27:DA:438:G:H2'   | 27:DA:440:G:H8    | 1.34                     | 0.91              |
| 31:DE:69:LYS:HD3  | 31:DE:89:ASP:HA   | 1.50                     | 0.91              |
| 1:AA:36:C:H5''    | 12:AL:119:THR:O   | 1.71                     | 0.91              |
| 3:AC:112:SER:HB3  | 3:AC:115:LEU:HD12 | 1.53                     | 0.91              |
| 3:CC:134:ILE:HG21 | 3:CC:168:ALA:HB3  | 1.53                     | 0.91              |
| 27:DA:579:G:H2'   | 27:DA:580:C:C6    | 2.06                     | 0.91              |
| 33:DG:43:LEU:HB2  | 33:DG:88:ILE:HD11 | 1.51                     | 0.91              |
| 27:BA:574:C:H42   | 31:BE:145:LYS:HE2 | 1.30                     | 0.90              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:BF:29:ASN:HB3  | 32:BF:112:MET:HE1  | 1.53                     | 0.90              |
| 38:BP:30:THR:HG22 | 38:BP:31:ALA:H     | 1.36                     | 0.90              |
| 1:CA:155:C:H2'    | 1:CA:156:G:H8      | 1.35                     | 0.90              |
| 10:CJ:32:ALA:HB2  | 10:CJ:76:ASN:HB2   | 1.52                     | 0.90              |
| 38:DP:63:PRO:CB   | 57:D8:13:ARG:HB3   | 2.01                     | 0.90              |
| 48:DZ:60:LEU:HB2  | 48:DZ:64:GLN:HB2   | 1.53                     | 0.90              |
| 27:BA:481:G:H1'   | 27:BA:506:G:H21    | 1.36                     | 0.90              |
| 27:DA:1747:G:H2'  | 27:DA:1747(A):G:H8 | 1.36                     | 0.90              |
| 27:BA:2879:C:H4'  | 27:BA:2880:C:OP1   | 1.68                     | 0.90              |
| 30:BD:186:HIS:HD2 | 30:BD:188:GLU:N    | 1.68                     | 0.90              |
| 31:BE:134:ILE:O   | 31:BE:134:ILE:HG12 | 1.71                     | 0.90              |
| 27:DA:2784:C:H1'  | 31:DE:37:ARG:HH12  | 1.34                     | 0.90              |
| 33:DG:5:VAL:HG23  | 33:DG:8:LYS:HG3    | 1.52                     | 0.90              |
| 47:DY:75:ILE:CG1  | 47:DY:79:CYS:HA    | 2.02                     | 0.90              |
| 15:AO:37:ASN:HD22 | 15:AO:37:ASN:N     | 1.68                     | 0.90              |
| 54:B5:4:HIS:HB3   | 54:B5:5:PRO:CD     | 2.01                     | 0.90              |
| 27:BA:1359:A:H2'  | 27:BA:1360:A:H5'   | 1.52                     | 0.90              |
| 27:BA:1636:C:H2'  | 27:BA:1637:A:C8    | 2.06                     | 0.90              |
| 30:BD:68:LYS:HZ1  | 30:BD:70:TRP:HE1   | 1.20                     | 0.90              |
| 7:CG:85:TYR:CD1   | 7:CG:154:TYR:HE1   | 1.90                     | 0.90              |
| 48:DZ:18:ARG:HB3  | 48:DZ:81:ARG:HH22  | 1.36                     | 0.90              |
| 1:AA:1162:C:H2'   | 1:AA:1163:C:H6     | 1.34                     | 0.90              |
| 8:AH:84:ARG:HG2   | 8:AH:84:ARG:HH11   | 1.37                     | 0.90              |
| 50:B1:46:LEU:HA   | 50:B1:63:ALA:HA    | 1.52                     | 0.90              |
| 54:B5:56:LYS:H    | 54:B5:56:LYS:HD2   | 1.35                     | 0.90              |
| 36:BN:115:ARG:HA  | 36:BN:118:LYS:HD2  | 1.52                     | 0.90              |
| 2:CB:14:GLY:O     | 2:CB:15:VAL:HG13   | 1.69                     | 0.90              |
| 7:CG:78:ARG:HG3   | 7:CG:79:ARG:H      | 1.35                     | 0.90              |
| 1:AA:473:G:H2'    | 1:AA:474:G:C8      | 2.05                     | 0.90              |
| 32:BF:8:GLN:HB3   | 32:BF:125:LEU:O    | 1.71                     | 0.90              |
| 14:CN:29:ARG:HG2  | 14:CN:40:CYS:HB2   | 1.53                     | 0.90              |
| 49:D0:26:TYR:H    | 49:D0:29:GLN:HE21  | 0.93                     | 0.90              |
| 32:DF:67:GLN:O    | 32:DF:67:GLN:HG3   | 1.72                     | 0.90              |
| 7:AG:113:GLU:CG   | 7:AG:119:ARG:HG2   | 2.01                     | 0.90              |
| 27:BA:360:G:H2'   | 27:BA:361:G:C8     | 2.06                     | 0.90              |
| 33:BG:42:GLY:O    | 33:BG:88:ILE:HD11  | 1.69                     | 0.90              |
| 30:DD:18:VAL:HG13 | 30:DD:211:ARG:HH22 | 1.36                     | 0.90              |
| 37:DO:17:ARG:HD3  | 37:DO:47:ILE:HD13  | 1.52                     | 0.90              |
| 27:DA:662:G:OP1   | 38:DP:18:ARG:HD2   | 1.71                     | 0.90              |
| 1:AA:62:U:H3      | 1:AA:105:G:H1      | 1.19                     | 0.90              |
| 51:B2:53:LEU:O    | 51:B2:57:ILE:HG12  | 1.72                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BX:12:VAL:HG23 | 46:BX:13:LEU:H    | 1.36                     | 0.90              |
| 47:BY:95:LYS:NZ   | 47:BY:100:ALA:HB2 | 1.85                     | 0.90              |
| 1:CA:179:A:H2'    | 1:CA:180:U:C6     | 2.07                     | 0.90              |
| 9:CI:26:VAL:HG22  | 9:CI:61:ALA:HB3   | 1.52                     | 0.90              |
| 38:DP:64:LYS:O    | 38:DP:66:GLY:N    | 2.05                     | 0.90              |
| 1:AA:358:U:H2'    | 1:AA:359:U:H6     | 1.37                     | 0.90              |
| 3:AC:113:ALA:HB3  | 3:AC:114:PRO:HD3  | 1.52                     | 0.90              |
| 17:AQ:57:VAL:HG12 | 17:AQ:76:LEU:HA   | 1.53                     | 0.90              |
| 1:AA:262:A:H5'    | 20:AT:74:LYS:HG3  | 1.52                     | 0.90              |
| 28:BB:40:U:N3     | 28:BB:43:C:H5''   | 1.87                     | 0.90              |
| 1:CA:161:A:H2'    | 1:CA:162:A:H8     | 1.34                     | 0.90              |
| 57:D8:52:LYS:N    | 57:D8:53:PRO:HD2  | 1.85                     | 0.90              |
| 27:DA:1461:G:H2'  | 27:DA:1462:C:H6   | 1.36                     | 0.90              |
| 27:DA:1681:G:OP2  | 27:DA:1681:G:H8   | 1.55                     | 0.90              |
| 27:DA:50:U:H4'    | 27:DA:51:G:OP2    | 1.71                     | 0.90              |
| 36:DN:76:SER:O    | 36:DN:78:TYR:N    | 2.05                     | 0.90              |
| 1:AA:271:C:H2'    | 1:AA:272:C:C6     | 2.06                     | 0.90              |
| 27:BA:1213:A:H8   | 27:BA:1213:A:H5'  | 1.33                     | 0.90              |
| 27:BA:1414:G:H1   | 27:BA:1588:C:H42  | 1.13                     | 0.90              |
| 41:BS:97:ARG:HH21 | 41:BS:98:VAL:HA   | 0.79                     | 0.90              |
| 1:CA:916:G:H2'    | 1:CA:917:G:H8     | 1.37                     | 0.90              |
| 3:CC:153:VAL:HG12 | 3:CC:196:LEU:HD11 | 1.51                     | 0.90              |
| 4:CD:9:CYS:HA     | 4:CD:12:CYS:HB2   | 1.54                     | 0.90              |
| 27:DA:1796:U:H2'  | 27:DA:1797:C:C6   | 2.05                     | 0.90              |
| 1:AA:1321:C:C5'   | 1:AA:1322:C:H5''  | 2.02                     | 0.89              |
| 1:AA:64:G:H4'     | 1:AA:65:U:O5'     | 1.71                     | 0.89              |
| 9:AI:53:VAL:HG23  | 9:AI:54:ASP:N     | 1.87                     | 0.89              |
| 17:AQ:87:LYS:HA   | 17:AQ:87:LYS:HE2  | 1.54                     | 0.89              |
| 20:AT:82:SER:O    | 20:AT:86:ARG:HB3  | 1.72                     | 0.89              |
| 27:BA:2876:G:H4'  | 42:BT:3:ARG:CD    | 2.02                     | 0.89              |
| 34:BH:85:LYS:HD2  | 34:BH:141:VAL:CG1 | 2.03                     | 0.89              |
| 41:BS:48:LEU:O    | 41:BS:49:VAL:HG23 | 1.71                     | 0.89              |
| 42:BT:41:ARG:O    | 42:BT:41:ARG:HD2  | 1.72                     | 0.89              |
| 47:BY:95:LYS:HZ3  | 47:BY:100:ALA:HB2 | 1.34                     | 0.89              |
| 47:BY:88:LYS:NZ   | 47:BY:93:GLY:HA3  | 1.86                     | 0.89              |
| 2:CB:204:ASN:ND2  | 2:CB:207:ALA:HB3  | 1.88                     | 0.89              |
| 9:CI:4:TYR:HB2    | 9:CI:19:LEU:HB2   | 1.53                     | 0.89              |
| 12:CL:43:LYS:CG   | 12:CL:44:LYS:H    | 1.85                     | 0.89              |
| 19:CS:49:ILE:HD12 | 19:CS:49:ILE:H    | 1.35                     | 0.89              |
| 29:DC:83:ILE:HG23 | 29:DC:94:VAL:HG23 | 1.52                     | 0.89              |
| 30:DD:31:LYS:O    | 30:DD:35:LYS:HB2  | 1.71                     | 0.89              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1249:U:H5'   | 27:BA:1249:U:C6    | 2.07                     | 0.89              |
| 28:BB:3:C:H42      | 28:BB:118:G:H1     | 1.04                     | 0.89              |
| 40:BR:98:LEU:HD12  | 40:BR:113:LEU:HD23 | 1.51                     | 0.89              |
| 42:BT:28:VAL:CG2   | 42:BT:47:GLY:H     | 1.85                     | 0.89              |
| 27:DA:2611:U:H1'   | 54:D5:3:LYS:HE3    | 1.54                     | 0.89              |
| 30:DD:10:THR:HG23  | 30:DD:13:ARG:HB3   | 1.54                     | 0.89              |
| 32:DF:7:TYR:HB2    | 32:DF:17:ARG:N     | 1.87                     | 0.89              |
| 34:DH:107:VAL:HG21 | 34:DH:152:ARG:HG2  | 1.54                     | 0.89              |
| 27:BA:1023:U:H2'   | 27:BA:1024:G:H5'   | 1.54                     | 0.89              |
| 27:BA:1596:A:C2'   | 27:BA:1597:A:H5'   | 2.02                     | 0.89              |
| 31:BE:8:LYS:HE3    | 31:BE:188:VAL:HG13 | 1.53                     | 0.89              |
| 34:BH:85:LYS:HZ2   | 34:BH:133:VAL:CG1  | 1.85                     | 0.89              |
| 1:CA:1398:A:H5''   | 1:CA:1398:A:H8     | 1.36                     | 0.89              |
| 20:CT:14:LYS:HB2   | 20:CT:17:ARG:HH21  | 1.33                     | 0.89              |
| 27:DA:1689:A:H62   | 27:DA:1698:A:H2    | 0.94                     | 0.89              |
| 27:DA:736:C:H42    | 27:DA:760:G:H1     | 1.20                     | 0.89              |
| 30:DD:61:LEU:HB3   | 30:DD:63:ARG:NH1   | 1.87                     | 0.89              |
| 1:AA:486:U:HO2'    | 1:AA:487:A:H8      | 0.92                     | 0.89              |
| 11:AK:48:ILE:HD11  | 11:AK:64:ALA:HA    | 1.53                     | 0.89              |
| 27:BA:1213:A:C8    | 27:BA:1213:A:H5'   | 2.07                     | 0.89              |
| 32:BF:2:LYS:H      | 32:BF:2:LYS:CD     | 1.85                     | 0.89              |
| 42:BT:125:ARG:O    | 42:BT:128:GLU:HG3  | 1.72                     | 0.89              |
| 45:BW:90:ARG:CB    | 45:BW:90:ARG:HH11  | 1.84                     | 0.89              |
| 27:BA:64:A:O3'     | 46:BX:71:GLY:HA3   | 1.71                     | 0.89              |
| 1:CA:99:U:H2'      | 1:CA:100:C:H6      | 1.36                     | 0.89              |
| 3:CC:43:LEU:HD13   | 3:CC:55:VAL:HG11   | 1.53                     | 0.89              |
| 27:DA:2161:C:H2'   | 27:DA:2162:G:C8    | 2.06                     | 0.89              |
| 28:DB:40:U:HO2'    | 28:DB:43:C:H5      | 0.92                     | 0.89              |
| 34:BH:43:VAL:HG11  | 34:BH:52:VAL:HG13  | 1.53                     | 0.89              |
| 39:BQ:134:ARG:HH21 | 48:BZ:121:ARG:CZ   | 1.83                     | 0.89              |
| 52:D3:23:LEU:HA    | 52:D3:26:LEU:HD12  | 1.54                     | 0.89              |
| 27:DA:2645:G:H4'   | 27:DA:2732:G:O2'   | 1.73                     | 0.89              |
| 31:DE:59:VAL:HG22  | 31:DE:60:ASN:H     | 1.35                     | 0.89              |
| 35:DI:144:VAL:HG23 | 35:DI:145:VAL:HG23 | 1.53                     | 0.89              |
| 1:AA:736:C:H2'     | 1:AA:737:A:C8      | 2.07                     | 0.89              |
| 57:B8:50:LEU:HD12  | 57:B8:51:ALA:H     | 1.36                     | 0.89              |
| 42:BT:89:VAL:CB    | 42:BT:91:ARG:HE    | 1.86                     | 0.89              |
| 10:CJ:48:THR:HG23  | 10:CJ:62:HIS:HB3   | 1.54                     | 0.89              |
| 12:CL:81:LEU:HD13  | 12:CL:82:ILE:H     | 1.35                     | 0.89              |
| 30:DD:118:VAL:HG22 | 30:DD:119:ALA:N    | 1.86                     | 0.89              |
| 27:DA:143(A):C:H4' | 46:DX:38:GLU:OE1   | 1.73                     | 0.89              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BP:59:LEU:HA    | 38:BP:61:ARG:NH1   | 1.86                     | 0.89              |
| 35:DI:75:LEU:HD21  | 35:DI:105:HIS:CE1  | 2.08                     | 0.89              |
| 1:AA:501:C:H2'     | 1:AA:502:G:H8      | 1.35                     | 0.89              |
| 13:AM:68:GLY:HA2   | 13:AM:71:ARG:HH21  | 1.37                     | 0.89              |
| 30:BD:13:ARG:NH1   | 30:BD:16:MET:SD    | 2.46                     | 0.89              |
| 43:BU:90:VAL:O     | 43:BU:92:ARG:N     | 2.05                     | 0.89              |
| 1:CA:1028:C:N4     | 1:CA:1034:G:H21    | 1.71                     | 0.89              |
| 6:CF:8:ILE:HG22    | 6:CF:10:LEU:HD11   | 1.53                     | 0.89              |
| 27:DA:125:G:H21    | 56:D7:48:LYS:HE3   | 1.36                     | 0.89              |
| 27:DA:2052:G:H21   | 31:DE:149:ARG:HA   | 1.36                     | 0.89              |
| 27:DA:2787:C:H1'   | 31:DE:61:ARG:CG    | 2.02                     | 0.89              |
| 27:BA:1884:A:C2'   | 27:BA:1885:A:H5''  | 2.02                     | 0.89              |
| 1:CA:922:G:H2'     | 1:CA:923:A:C8      | 2.08                     | 0.89              |
| 1:CA:750:G:N3      | 15:CO:23:GLY:HA3   | 1.88                     | 0.89              |
| 23:CW:35:G:HO2'    | 23:CW:36:A:H8      | 1.21                     | 0.89              |
| 27:DA:1416:G:HO2'  | 27:DA:1417:C:H6    | 0.92                     | 0.89              |
| 28:DB:7:G:H2'      | 28:DB:8:U:H5''     | 1.53                     | 0.89              |
| 38:DP:105:LEU:O    | 38:DP:106:LEU:HB2  | 1.70                     | 0.89              |
| 38:DP:45:LEU:CD2   | 38:DP:46:LYS:H     | 1.84                     | 0.89              |
| 42:DT:88:ILE:HG22  | 42:DT:89:VAL:N     | 1.83                     | 0.89              |
| 1:AA:70:G:H1       | 1:AA:99:U:H3       | 1.21                     | 0.89              |
| 11:AK:50:TYR:HB3   | 11:AK:54:ARG:O     | 1.73                     | 0.89              |
| 27:BA:1246:A:OP2   | 38:BP:18:ARG:HG3   | 1.73                     | 0.89              |
| 31:BE:78:LEU:HD23  | 31:BE:78:LEU:N     | 1.88                     | 0.89              |
| 42:BT:68:TYR:O     | 42:BT:70:VAL:N     | 2.04                     | 0.89              |
| 27:DA:1504:C:C2'   | 27:DA:1505:C:H5''  | 2.03                     | 0.89              |
| 27:DA:2150:U:H2'   | 27:DA:2151:G:H8    | 1.38                     | 0.89              |
| 48:DZ:52:ILE:HG21  | 48:DZ:70:VAL:O     | 1.71                     | 0.89              |
| 12:AL:73:ASN:ND2   | 12:AL:74:LEU:H     | 1.68                     | 0.88              |
| 34:BH:113:VAL:HG21 | 34:BH:151:ILE:HG21 | 1.55                     | 0.88              |
| 38:BP:23:PRO:HB3   | 38:BP:29:LYS:HB2   | 1.55                     | 0.88              |
| 49:D0:41:ARG:CD    | 49:D0:41:ARG:H     | 1.86                     | 0.88              |
| 38:DP:41:ARG:HE    | 38:DP:41:ARG:HA    | 1.38                     | 0.88              |
| 39:DQ:81:VAL:HG21  | 49:D0:7:LEU:HD21   | 1.54                     | 0.88              |
| 11:AK:127:LYS:CE   | 11:AK:127:LYS:HA   | 2.03                     | 0.88              |
| 12:AL:38:ARG:HH12  | 12:AL:54:LYS:NZ    | 1.71                     | 0.88              |
| 27:BA:2516:G:C2'   | 27:BA:2517:C:H5'   | 2.03                     | 0.88              |
| 38:BP:107:LYS:O    | 38:BP:109:GLY:N    | 2.06                     | 0.88              |
| 3:AC:16:ARG:HH11   | 3:AC:16:ARG:HB2    | 1.34                     | 0.88              |
| 27:BA:1291:C:H2'   | 27:BA:1292:U:H6    | 1.37                     | 0.88              |
| 30:BD:165:ILE:HD13 | 30:BD:175:LEU:CD2  | 2.03                     | 0.88              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BH:85:LYS:HD2  | 34:BH:141:VAL:HG12 | 1.53                     | 0.88              |
| 35:BI:38:LEU:HD12 | 35:BI:38:LEU:H     | 1.36                     | 0.88              |
| 37:BO:10:VAL:HG21 | 37:BO:16:ALA:O     | 1.74                     | 0.88              |
| 1:CA:250:A:H4'    | 1:CA:251:G:O5'     | 1.71                     | 0.88              |
| 10:CJ:8:LEU:HD21  | 10:CJ:96:ILE:HG22  | 1.55                     | 0.88              |
| 57:D8:10:ALA:HB3  | 57:D8:60:LEU:HD21  | 1.55                     | 0.88              |
| 27:DA:1146:C:O2'  | 27:DA:1147:C:H5'   | 1.74                     | 0.88              |
| 27:DA:2887:U:H2'  | 27:DA:2888:C:H6    | 1.37                     | 0.88              |
| 27:DA:1826:G:C4'  | 30:DD:242:ARG:HH21 | 1.86                     | 0.88              |
| 5:AE:76:ILE:HG13  | 5:AE:77:PRO:HD2    | 1.53                     | 0.88              |
| 23:AW:66:A:H2'    | 23:AW:67:C:C6      | 2.09                     | 0.88              |
| 51:B2:41:ILE:HG13 | 51:B2:42:GLY:O     | 1.72                     | 0.88              |
| 27:BA:1292:U:H2'  | 27:BA:1293:C:H6    | 1.38                     | 0.88              |
| 2:CB:98:LEU:O     | 2:CB:101:MET:HG3   | 1.72                     | 0.88              |
| 5:CE:11:ILE:HG22  | 5:CE:12:LEU:H      | 1.39                     | 0.88              |
| 47:DY:96:ILE:HD12 | 47:DY:99:CYS:SG    | 2.13                     | 0.88              |
| 12:AL:33:VAL:O    | 12:AL:55:VAL:HG13  | 1.74                     | 0.88              |
| 1:AA:736:C:H5''   | 18:AR:72:ARG:HH21  | 1.36                     | 0.88              |
| 27:BA:1296:G:O2'  | 27:BA:1297:C:H5'   | 1.73                     | 0.88              |
| 27:BA:845:G:H4'   | 27:BA:846:C:OP1    | 1.73                     | 0.88              |
| 42:BT:65:LYS:NZ   | 42:BT:66:VAL:HG23  | 1.88                     | 0.88              |
| 1:CA:351:G:H4'    | 1:CA:352:C:OP1     | 1.74                     | 0.88              |
| 55:D6:32:ASN:ND2  | 55:D6:33:LYS:H     | 1.72                     | 0.88              |
| 27:DA:1504:C:H2'  | 27:DA:1505:C:H5''  | 1.53                     | 0.88              |
| 27:DA:2550:G:H22  | 27:DA:2559:C:H1'   | 1.39                     | 0.88              |
| 27:DA:908:C:H3'   | 39:DQ:22:LYS:NZ    | 1.89                     | 0.88              |
| 33:DG:39:ILE:HG23 | 33:DG:92:VAL:HG13  | 1.55                     | 0.88              |
| 38:DP:38:GLN:HG3  | 38:DP:39:LYS:H     | 1.37                     | 0.88              |
| 27:DA:2683:C:P    | 42:DT:53:ARG:HH22  | 1.96                     | 0.88              |
| 27:BA:197:A:H5'   | 27:BA:197:A:H8     | 1.35                     | 0.88              |
| 27:BA:2694:G:H8   | 27:BA:2694:G:H5'   | 1.39                     | 0.88              |
| 12:CL:81:LEU:HD13 | 12:CL:82:ILE:N     | 1.87                     | 0.88              |
| 49:D0:26:TYR:N    | 49:D0:29:GLN:HE21  | 1.71                     | 0.88              |
| 32:DF:36:VAL:HG11 | 32:DF:183:VAL:HG21 | 1.53                     | 0.88              |
| 42:DT:118:ARG:HA  | 42:DT:121:ILE:HB   | 1.55                     | 0.88              |
| 1:AA:1137:C:H4'   | 1:AA:1138:G:C2     | 2.08                     | 0.88              |
| 14:AN:6:LEU:HD13  | 14:AN:23:ARG:HH22  | 1.34                     | 0.88              |
| 31:BE:132:HIS:O   | 31:BE:133:LYS:HG3  | 1.73                     | 0.88              |
| 34:BH:20:ALA:HB1  | 34:BH:21:PRO:HD2   | 1.54                     | 0.88              |
| 38:BP:85:LEU:HD21 | 38:BP:116:GLY:O    | 1.73                     | 0.88              |
| 43:BU:91:ASP:OD2  | 43:BU:96:ALA:HB2   | 1.72                     | 0.88              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:904:C:H2'    | 27:DA:905:U:H5'    | 1.52                     | 0.88              |
| 42:DT:99:LEU:HB2   | 42:DT:101:PHE:HE1  | 1.38                     | 0.88              |
| 16:AP:22:THR:OG1   | 16:AP:26:ARG:HG3   | 1.72                     | 0.88              |
| 27:BA:2657:A:O2'   | 34:BH:160:LYS:HE3  | 1.73                     | 0.88              |
| 27:BA:805:G:H4'    | 27:BA:806:C:OP2    | 1.71                     | 0.88              |
| 34:BH:10:PRO:HG3   | 34:BH:50:VAL:O     | 1.73                     | 0.88              |
| 1:CA:838:G:H2'     | 1:CA:839:U:H5''    | 1.55                     | 0.88              |
| 2:CB:178:ARG:NH2   | 8:CH:68:ARG:HH22   | 1.71                     | 0.88              |
| 25:CY:68:C:H2'     | 25:CY:69:C:H5''    | 1.55                     | 0.88              |
| 27:DA:1658:C:OP1   | 31:DE:132:HIS:ND1  | 2.07                     | 0.88              |
| 4:AD:196:LEU:N     | 4:AD:196:LEU:HD12  | 1.89                     | 0.88              |
| 57:B8:43:GLN:C     | 57:B8:44:LYS:HD2   | 1.94                     | 0.88              |
| 1:CA:1502:A:H4'    | 1:CA:1503:A:OP2    | 1.72                     | 0.88              |
| 25:CY:2:G:H1       | 25:CY:70:C:H42     | 1.17                     | 0.88              |
| 27:DA:630:G:H1     | 27:DA:634:C:N4     | 1.71                     | 0.88              |
| 27:DA:676:A:H2     | 27:DA:802:A:H61    | 1.22                     | 0.88              |
| 54:B5:16:ARG:HG2   | 54:B5:16:ARG:NH1   | 1.81                     | 0.88              |
| 27:BA:2283:C:H2'   | 27:BA:2284:C:H5'   | 1.56                     | 0.88              |
| 36:BN:30:ILE:HG23  | 36:BN:52:VAL:HG11  | 1.56                     | 0.88              |
| 3:CC:95:THR:HG22   | 3:CC:97:LYS:HB2    | 1.53                     | 0.88              |
| 27:DA:2296:U:H4'   | 27:DA:2297:C:OP1   | 1.74                     | 0.88              |
| 27:DA:271(H):G:H2' | 27:DA:271(I):G:H8  | 1.38                     | 0.88              |
| 27:DA:690:G:H2'    | 27:DA:691:C:C6     | 2.09                     | 0.88              |
| 38:DP:101:VAL:HG12 | 38:DP:106:LEU:HD23 | 1.56                     | 0.88              |
| 39:DQ:42:ILE:HD13  | 39:DQ:97:VAL:HG21  | 1.56                     | 0.88              |
| 46:DX:12:VAL:HG13  | 46:DX:27:THR:O     | 1.73                     | 0.88              |
| 4:AD:127:THR:HB    | 4:AD:130:GLY:O     | 1.74                     | 0.87              |
| 27:BA:1372:U:H2'   | 27:BA:1373:A:C8    | 2.08                     | 0.87              |
| 27:BA:2524:G:H5'   | 27:BA:2525:G:OP2   | 1.73                     | 0.87              |
| 37:BO:119:PRO:O    | 37:BO:120:GLU:HB3  | 1.71                     | 0.87              |
| 42:BT:28:VAL:HG22  | 42:BT:47:GLY:H     | 1.38                     | 0.87              |
| 1:CA:1226:C:C5     | 13:CM:104:ARG:HA   | 2.09                     | 0.87              |
| 1:CA:1315:U:H2'    | 1:CA:1316:G:O4'    | 1.74                     | 0.87              |
| 19:CS:48:THR:HG22  | 19:CS:61:TYR:HA    | 1.55                     | 0.87              |
| 27:DA:142:A:C8     | 27:DA:1408:C:H1'   | 2.09                     | 0.87              |
| 34:DH:44:VAL:HG12  | 34:DH:45:VAL:H     | 1.39                     | 0.87              |
| 39:DQ:55:VAL:HG13  | 39:DQ:56:ARG:H     | 1.39                     | 0.87              |
| 27:BA:2189:U:H3'   | 27:BA:2190:G:H5''  | 1.56                     | 0.87              |
| 37:BO:104:ARG:HH12 | 42:BT:35:LYS:CE    | 1.87                     | 0.87              |
| 1:CA:1157:A:H4'    | 1:CA:1158:C:O5'    | 1.74                     | 0.87              |
| 27:DA:806:C:OP2    | 38:DP:39:LYS:HD3   | 1.75                     | 0.87              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1285:A:H4'   | 1:AA:1286:A:O5'    | 1.74                     | 0.87              |
| 30:BD:246:PRO:HG2 | 30:BD:255:LYS:HG3  | 1.56                     | 0.87              |
| 31:BE:59:VAL:CG2  | 31:BE:60:ASN:H     | 1.87                     | 0.87              |
| 34:BH:86:GLU:HB2  | 34:BH:132:ARG:HH12 | 1.38                     | 0.87              |
| 42:BT:13:ARG:HA   | 42:BT:13:ARG:CZ    | 2.04                     | 0.87              |
| 44:BV:15:GLU:HB3  | 44:BV:16:PRO:HD2   | 1.57                     | 0.87              |
| 27:DA:1410:G:H2'  | 27:DA:1411:C:H6    | 1.34                     | 0.87              |
| 27:DA:1449:A:C2   | 27:DA:1450:G:H1'   | 2.08                     | 0.87              |
| 27:DA:574:C:H1'   | 27:DA:2055:C:C6    | 2.09                     | 0.87              |
| 34:DH:126:PRO:O   | 34:DH:127:GLU:HB2  | 1.75                     | 0.87              |
| 41:DS:34:HIS:CE1  | 41:DS:54:LEU:HB2   | 2.08                     | 0.87              |
| 38:BP:23:PRO:HB2  | 38:BP:33:ARG:HG3   | 1.56                     | 0.87              |
| 45:BW:76:VAL:HB   | 45:BW:103:ILE:HG23 | 1.57                     | 0.87              |
| 55:D6:32:ASN:HD22 | 55:D6:33:LYS:H     | 0.87                     | 0.87              |
| 27:DA:748:G:H5'   | 45:DW:89:ALA:HB2   | 1.54                     | 0.87              |
| 32:DF:25:PRO:HG3  | 32:DF:119:ARG:HB2  | 1.56                     | 0.87              |
| 44:DV:66:ARG:HH21 | 44:DV:88:ARG:HD3   | 1.39                     | 0.87              |
| 1:AA:1002:G:H21   | 1:AA:1003:G:H1'    | 1.40                     | 0.87              |
| 1:AA:1004:A:H5''  | 1:AA:1025:U:H3     | 1.38                     | 0.87              |
| 38:BP:23:PRO:HD2  | 38:BP:33:ARG:CZ    | 2.04                     | 0.87              |
| 42:BT:91:ARG:HA   | 42:BT:117:ASP:H    | 1.39                     | 0.87              |
| 27:DA:2475:C:H42  | 27:DA:2529:G:N2    | 1.72                     | 0.87              |
| 47:DY:28:LYS:CB   | 47:DY:39:VAL:H     | 1.87                     | 0.87              |
| 27:BA:2439:A:H5'  | 27:BA:2439:A:C8    | 2.09                     | 0.87              |
| 1:CA:452:A:O2'    | 1:CA:453:A:H5''    | 1.74                     | 0.87              |
| 4:CD:9:CYS:SG     | 4:CD:31:CYS:O      | 2.33                     | 0.87              |
| 12:CL:80:VAL:HG12 | 12:CL:81:LEU:H     | 1.39                     | 0.87              |
| 19:CS:32:LYS:HE3  | 19:CS:32:LYS:H     | 1.39                     | 0.87              |
| 4:AD:149:ALA:HB3  | 4:AD:152:SER:HB2   | 1.54                     | 0.87              |
| 13:AM:86:CYS:HB2  | 19:AS:73:GLU:HB3   | 1.54                     | 0.87              |
| 27:BA:1378:A:H4'  | 27:BA:1379:A:OP1   | 1.73                     | 0.87              |
| 14:CN:23:ARG:HD2  | 14:CN:28:GLY:O     | 1.72                     | 0.87              |
| 27:DA:2883:A:H3'  | 27:DA:2884:U:H5'   | 1.54                     | 0.87              |
| 27:DA:519:U:H2'   | 27:DA:520:G:H8     | 1.32                     | 0.87              |
| 1:AA:1399:C:H4'   | 1:AA:1400:C:O5'    | 1.74                     | 0.87              |
| 17:AQ:26:GLN:HB3  | 17:AQ:37:LYS:HG2   | 1.57                     | 0.87              |
| 27:BA:480:A:C1'   | 47:BY:44:ILE:HG21  | 2.04                     | 0.87              |
| 37:BO:78:ARG:HH11 | 37:BO:78:ARG:HB2   | 1.37                     | 0.87              |
| 27:DA:1403:C:H5'' | 27:DA:1471:A:H1'   | 1.57                     | 0.87              |
| 30:DD:270:ILE:O   | 30:DD:271:ILE:HG23 | 1.74                     | 0.87              |
| 31:DE:4:ILE:HG12  | 31:DE:28:ALA:HB1   | 1.57                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DG:111:LEU:HD11 | 33:DG:120:LEU:HD21 | 1.57                     | 0.87              |
| 42:DT:105:LEU:HD13 | 42:DT:109:GLU:OE2  | 1.75                     | 0.87              |
| 1:AA:577:G:HO2'    | 1:AA:578:C:H6      | 0.91                     | 0.87              |
| 2:AB:219:VAL:HA    | 2:AB:222:ILE:HD12  | 1.55                     | 0.87              |
| 19:AS:49:ILE:HD12  | 19:AS:49:ILE:H     | 1.40                     | 0.87              |
| 27:BA:2516:G:O2'   | 27:BA:2517:C:H5'   | 1.75                     | 0.87              |
| 27:BA:626:U:H5'    | 27:BA:627:A:H5'    | 1.55                     | 0.87              |
| 27:BA:2128:C:OP1   | 29:BC:35:ALA:HB1   | 1.75                     | 0.87              |
| 41:BS:89:ARG:O     | 41:BS:92:TYR:HB3   | 1.72                     | 0.87              |
| 48:BZ:119:ILE:O    | 48:BZ:120:HIS:HB2  | 1.75                     | 0.87              |
| 13:CM:68:GLY:O     | 13:CM:71:ARG:HB3   | 1.73                     | 0.87              |
| 27:DA:2526:G:H21   | 58:D9:2:LYS:HG3    | 1.38                     | 0.87              |
| 27:DA:2150:U:H2'   | 27:DA:2151:G:C8    | 2.10                     | 0.87              |
| 42:DT:96:ARG:HG2   | 42:DT:96:ARG:HH11  | 1.40                     | 0.87              |
| 47:DY:27:VAL:HG12  | 47:DY:28:LYS:H     | 1.38                     | 0.87              |
| 1:AA:815:A:H5''    | 1:AA:817:C:N4      | 1.90                     | 0.86              |
| 27:BA:2271:G:H4'   | 49:B0:20:ARG:HH12  | 1.40                     | 0.86              |
| 27:BA:754:C:H2'    | 27:BA:755:C:H6     | 1.38                     | 0.86              |
| 33:BG:82:LEU:HD22  | 33:BG:87:PRO:HG3   | 1.53                     | 0.86              |
| 36:BN:1:MET:HG2    | 36:BN:2:LYS:N      | 1.86                     | 0.86              |
| 37:BO:65:THR:HA    | 37:BO:82:ASN:HD22  | 1.40                     | 0.86              |
| 1:CA:601:C:H2'     | 1:CA:602:A:H8      | 1.37                     | 0.86              |
| 25:CY:17:G:H22     | 25:CY:54:U:H1'     | 1.39                     | 0.86              |
| 27:DA:272(C):G:H1  | 27:DA:365:C:H42    | 1.22                     | 0.86              |
| 27:DA:863:A:H2'    | 27:DA:864:G:C8     | 2.09                     | 0.86              |
| 31:DE:77:ILE:CG2   | 31:DE:78:LEU:H     | 1.78                     | 0.86              |
| 37:DO:80:ASP:OD2   | 42:DT:71:GLY:HA3   | 1.75                     | 0.86              |
| 1:AA:1278:U:H5''   | 1:AA:1279:A:H5'    | 1.56                     | 0.86              |
| 3:AC:59:ARG:HG2    | 3:AC:63:ASN:O      | 1.74                     | 0.86              |
| 27:BA:271(Q):G:H2' | 27:BA:271(R):G:C8  | 2.10                     | 0.86              |
| 27:BA:2723:C:H5'   | 40:BR:5:LYS:HZ2    | 1.37                     | 0.86              |
| 1:CA:1154:G:HO2'   | 1:CA:1155:G:H8     | 0.88                     | 0.86              |
| 9:CI:97:LYS:HB3    | 9:CI:98:PRO:HD3    | 1.57                     | 0.86              |
| 1:CA:718:G:H21     | 18:CR:49:LYS:NZ    | 1.73                     | 0.86              |
| 27:DA:2619:C:H5''  | 31:DE:152:LYS:HA   | 1.55                     | 0.86              |
| 4:AD:9:CYS:H       | 4:AD:22:LYS:HZ3    | 1.24                     | 0.86              |
| 38:BP:71:VAL:HG12  | 38:BP:72:PRO:HD3   | 1.56                     | 0.86              |
| 42:BT:104:ASN:O    | 42:BT:105:LEU:HD23 | 1.75                     | 0.86              |
| 1:CA:1065:U:H5''   | 1:CA:1190:G:H21    | 1.39                     | 0.86              |
| 5:CE:91:LEU:HG     | 5:CE:120:THR:HG22  | 1.54                     | 0.86              |
| 27:DA:1019:U:H3    | 27:DA:1142(A):A:N6 | 1.73                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:200:U:H5'   | 27:DA:200:U:C6    | 2.10                     | 0.86              |
| 27:DA:2612:C:O2'  | 27:DA:2613:U:H5'  | 1.76                     | 0.86              |
| 27:DA:2645:G:H4'  | 27:DA:2732:G:HO2' | 1.40                     | 0.86              |
| 30:DD:242:ARG:N   | 30:DD:242:ARG:HD2 | 1.88                     | 0.86              |
| 39:DQ:12:GLN:NE2  | 39:DQ:72:LYS:HG3  | 1.89                     | 0.86              |
| 42:DT:14:TYR:H    | 42:DT:14:TYR:HD1  | 1.23                     | 0.86              |
| 12:AL:29:PHE:HB3  | 12:AL:81:LEU:CD1  | 2.05                     | 0.86              |
| 27:BA:1474:C:H2'  | 27:BA:1475:G:H8   | 1.37                     | 0.86              |
| 30:BD:267:SER:O   | 30:BD:269:PHE:N   | 2.09                     | 0.86              |
| 39:BQ:111:GLU:O   | 39:BQ:115:MET:HB2 | 1.76                     | 0.86              |
| 1:CA:838:G:C2'    | 1:CA:839:U:H5''   | 2.06                     | 0.86              |
| 3:CC:156:ARG:HH21 | 3:CC:161:GLU:HG3  | 1.40                     | 0.86              |
| 7:CG:150:ALA:HB2  | 11:CK:50:TYR:OH   | 1.75                     | 0.86              |
| 11:CK:111:ASP:HA  | 18:CR:84:LYS:HG3  | 1.57                     | 0.86              |
| 41:DS:89:ARG:HB3  | 41:DS:92:TYR:HB3  | 1.57                     | 0.86              |
| 9:AI:82:ALA:HA    | 9:AI:85:LEU:HD11  | 1.56                     | 0.86              |
| 27:BA:1173:G:H3'  | 27:BA:1174:A:C5'  | 2.02                     | 0.86              |
| 27:BA:2138:C:H2'  | 27:BA:2139:C:H6   | 1.39                     | 0.86              |
| 32:BF:181:LEU:HB3 | 32:BF:205:ARG:NH1 | 1.90                     | 0.86              |
| 34:BH:97:ARG:HG2  | 34:BH:98:LEU:H    | 1.40                     | 0.86              |
| 36:BN:4:TYR:CD1   | 36:BN:4:TYR:N     | 2.39                     | 0.86              |
| 43:BU:88:ILE:HG22 | 44:BV:47:VAL:HG23 | 1.57                     | 0.86              |
| 1:CA:471:G:O2'    | 1:CA:472:A:H8     | 1.58                     | 0.86              |
| 23:CW:20:A:N6     | 23:CW:46:U:H1'    | 1.89                     | 0.86              |
| 27:DA:2880:C:O2'  | 40:DR:90:ARG:HD3  | 1.75                     | 0.86              |
| 38:DP:78:PRO:HB2  | 38:DP:111:ARG:HD2 | 1.57                     | 0.86              |
| 3:AC:83:ARG:O     | 3:AC:86:VAL:HG22  | 1.76                     | 0.86              |
| 23:AW:30:A:C2'    | 23:AW:31:U:H5''   | 2.04                     | 0.86              |
| 27:BA:1577:C:H2'  | 27:BA:1578:U:C6   | 2.09                     | 0.86              |
| 27:BA:2505:G:O2'  | 27:BA:2506:U:H5'  | 1.76                     | 0.86              |
| 37:BO:20:MET:O    | 37:BO:41:ALA:HB1  | 1.75                     | 0.86              |
| 48:BZ:52:ILE:CG2  | 48:BZ:70:VAL:HB   | 2.06                     | 0.86              |
| 11:CK:32:ILE:CD1  | 11:CK:72:ALA:HB2  | 2.04                     | 0.86              |
| 13:CM:23:TYR:HB3  | 13:CM:67:GLU:HB2  | 1.57                     | 0.86              |
| 27:DA:830:G:H4'   | 27:DA:831:G:OP2   | 1.74                     | 0.86              |
| 27:DA:969:U:OP1   | 52:D3:17:LYS:HG2  | 1.75                     | 0.86              |
| 32:DF:109:GLY:HA2 | 32:DF:112:MET:HB3 | 1.57                     | 0.86              |
| 41:DS:17:ARG:O    | 41:DS:18:ILE:HB   | 1.72                     | 0.86              |
| 2:AB:18:GLY:N     | 2:AB:42:ILE:HG22  | 1.89                     | 0.86              |
| 6:AF:67:MET:HB2   | 6:AF:68:PRO:HD2   | 1.56                     | 0.86              |
| 55:B6:40:CYS:CA   | 55:B6:46:HIS:HB3  | 2.06                     | 0.86              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 58:B9:29:ASN:N     | 58:B9:29:ASN:HD22 | 1.71                     | 0.86              |
| 27:BA:2876:G:H4'   | 42:BT:3:ARG:HD3   | 1.58                     | 0.86              |
| 44:BV:19:LYS:HE2   | 44:BV:20:LEU:N    | 1.91                     | 0.86              |
| 46:BX:12:VAL:HG13  | 46:BX:27:THR:O    | 1.74                     | 0.86              |
| 12:CL:3:THR:O      | 12:CL:7:LEU:HD12  | 1.74                     | 0.86              |
| 36:DN:57:ALA:HB3   | 36:DN:124:ALA:HA  | 1.58                     | 0.86              |
| 40:DR:10:LEU:HB3   | 40:DR:17:ARG:NE   | 1.91                     | 0.86              |
| 1:AA:631:G:H5''    | 1:AA:632:A:OP1    | 1.75                     | 0.86              |
| 2:AB:178:ARG:HH22  | 2:AB:196:LEU:HA   | 1.40                     | 0.86              |
| 3:AC:129:ALA:HB3   | 3:AC:132:ARG:HB3  | 1.58                     | 0.86              |
| 13:AM:7:VAL:HG12   | 13:AM:9:ILE:HD11  | 1.58                     | 0.86              |
| 27:BA:109:G:O2'    | 27:BA:110:G:H5'   | 1.75                     | 0.86              |
| 27:BA:1336:A:H2'   | 27:BA:1337:G:C8   | 2.09                     | 0.86              |
| 27:BA:2200:C:H2'   | 27:BA:2201:C:H6   | 1.41                     | 0.86              |
| 27:BA:271(F):C:H42 | 27:BA:271(R):G:H1 | 1.22                     | 0.86              |
| 27:BA:2723:C:H5'   | 40:BR:5:LYS:NZ    | 1.91                     | 0.86              |
| 50:D1:11:ARG:HB2   | 50:D1:12:PRO:HD2  | 1.55                     | 0.86              |
| 27:DA:8:A:H2'      | 27:DA:9:U:C6      | 2.11                     | 0.86              |
| 27:BA:2090:G:N2    | 50:B1:45:ASN:HD21 | 1.74                     | 0.86              |
| 27:BA:2199:A:C8    | 27:BA:2199:A:H5'  | 2.10                     | 0.86              |
| 27:BA:795:C:H2'    | 27:BA:796:C:C6    | 2.11                     | 0.86              |
| 47:BY:96:ILE:HG22  | 47:BY:97:ARG:N    | 1.89                     | 0.86              |
| 13:CM:3:ARG:HG2    | 13:CM:9:ILE:CG1   | 2.05                     | 0.86              |
| 27:DA:2467:C:H4'   | 39:DQ:123:HIS:CD2 | 2.11                     | 0.86              |
| 33:DG:39:ILE:CG2   | 33:DG:92:VAL:HG13 | 2.06                     | 0.86              |
| 34:DH:53:GLU:O     | 34:DH:54:ARG:HB3  | 1.73                     | 0.86              |
| 35:DI:37:VAL:HG12  | 35:DI:38:LEU:H    | 1.40                     | 0.86              |
| 9:AI:53:VAL:CG2    | 9:AI:54:ASP:H     | 1.88                     | 0.86              |
| 9:AI:50:LEU:HB3    | 9:AI:55:ALA:O     | 1.76                     | 0.86              |
| 40:BR:24:GLN:HE21  | 40:BR:36:THR:HG21 | 1.40                     | 0.86              |
| 42:BT:65:LYS:CE    | 42:BT:66:VAL:H    | 1.88                     | 0.86              |
| 1:CA:234:C:H2'     | 1:CA:235:C:C6     | 2.09                     | 0.86              |
| 10:CJ:34:VAL:HG22  | 10:CJ:74:ILE:HG22 | 1.55                     | 0.86              |
| 11:CK:127:LYS:HA   | 11:CK:127:LYS:HE2 | 1.58                     | 0.86              |
| 27:DA:1273:U:H6    | 27:DA:1273:U:H5'' | 1.39                     | 0.86              |
| 27:DA:1718:G:H1    | 27:DA:1744:C:H42  | 1.24                     | 0.86              |
| 27:DA:2756:U:H1'   | 27:DA:2757:A:H5'' | 1.57                     | 0.86              |
| 27:DA:560:C:H4'    | 43:DU:52:ARG:NH2  | 1.90                     | 0.86              |
| 1:AA:1162:C:H2'    | 1:AA:1163:C:C6    | 2.11                     | 0.85              |
| 1:AA:1270:C:O2'    | 1:AA:1271:G:H5'   | 1.74                     | 0.85              |
| 27:BA:200:U:H5'    | 27:BA:200:U:H6    | 1.40                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2571:C:H5'   | 27:BA:2572:A:H5''  | 1.58                     | 0.85              |
| 27:BA:2863:C:H2'   | 27:BA:2864:G:H5''  | 1.55                     | 0.85              |
| 30:BD:71:ASP:HB2   | 30:BD:103:ARG:HH22 | 1.38                     | 0.85              |
| 1:CA:1173:G:H2'    | 1:CA:1174:G:H8     | 1.41                     | 0.85              |
| 1:CA:1270:C:O2'    | 1:CA:1271:G:H5'    | 1.76                     | 0.85              |
| 1:CA:566:G:H4'     | 1:CA:567:G:OP1     | 1.76                     | 0.85              |
| 8:CH:42:GLU:HG3    | 8:CH:109:ILE:HD12  | 1.56                     | 0.85              |
| 14:CN:13:THR:N     | 14:CN:14:PRO:HD2   | 1.89                     | 0.85              |
| 27:DA:869:G:H2'    | 27:DA:870:A:C8     | 2.09                     | 0.85              |
| 34:DH:13:LYS:HA    | 34:DH:13:LYS:HE2   | 1.58                     | 0.85              |
| 10:AJ:46:ARG:HG2   | 10:AJ:64:GLU:OE1   | 1.74                     | 0.85              |
| 55:B6:19:ARG:H     | 55:B6:19:ARG:HD2   | 1.39                     | 0.85              |
| 57:B8:6:THR:HA     | 57:B8:61:LEU:HD11  | 1.58                     | 0.85              |
| 27:BA:1562:A:H2'   | 27:BA:1563:G:H8    | 1.38                     | 0.85              |
| 27:BA:2071:A:H2    | 27:BA:2441:C:N3    | 1.72                     | 0.85              |
| 30:BD:35:LYS:HZ3   | 30:BD:103:ARG:HA   | 1.40                     | 0.85              |
| 34:BH:92:ILE:HG22  | 34:BH:93:GLY:N     | 1.89                     | 0.85              |
| 1:CA:1208:C:H2'    | 1:CA:1209:C:C6     | 2.10                     | 0.85              |
| 8:CH:109:ILE:HG12  | 8:CH:110:ALA:H     | 1.41                     | 0.85              |
| 15:CO:16:ALA:HB1   | 15:CO:21:ASP:HB3   | 1.57                     | 0.85              |
| 16:CP:5:ARG:HH12   | 16:CP:24:ALA:HA    | 1.40                     | 0.85              |
| 23:CW:20:A:H62     | 23:CW:44:A:H2'     | 1.41                     | 0.85              |
| 27:DA:2100:G:H2'   | 27:DA:2101:G:C8    | 2.10                     | 0.85              |
| 27:DA:2752:C:H2'   | 27:DA:2753:A:C8    | 2.11                     | 0.85              |
| 28:DB:7:G:H5'      | 41:DS:29:PHE:CE1   | 2.11                     | 0.85              |
| 46:DX:24:GLY:O     | 46:DX:82:GLN:HA    | 1.76                     | 0.85              |
| 8:CH:95:VAL:HA     | 8:CH:99:GLU:OE2    | 1.77                     | 0.85              |
| 56:D7:9:ARG:HB3    | 56:D7:48:LYS:NZ    | 1.91                     | 0.85              |
| 57:D8:6:THR:HG22   | 57:D8:63:PRO:CD    | 2.07                     | 0.85              |
| 27:DA:184:C:H2'    | 27:DA:185:U:H6     | 1.41                     | 0.85              |
| 30:DD:239:ARG:HH21 | 30:DD:239:ARG:CG   | 1.88                     | 0.85              |
| 32:DF:186:ILE:HG23 | 32:DF:192:LEU:HD11 | 1.58                     | 0.85              |
| 8:AH:6:ILE:H       | 8:AH:6:ILE:HD12    | 1.39                     | 0.85              |
| 19:AS:63:THR:HG22  | 19:AS:66:MET:CE    | 2.07                     | 0.85              |
| 49:B0:10:THR:HG23  | 49:B0:12:ASN:OD1   | 1.77                     | 0.85              |
| 27:BA:491:G:H2'    | 27:BA:492:A:H8     | 1.40                     | 0.85              |
| 36:BN:1:MET:HG2    | 36:BN:2:LYS:H      | 1.38                     | 0.85              |
| 46:BX:39:ILE:O     | 46:BX:43:VAL:HG23  | 1.76                     | 0.85              |
| 1:CA:1356:G:H1     | 1:CA:1366:C:H42    | 1.24                     | 0.85              |
| 27:DA:232:G:H4'    | 27:DA:233:A:OP1    | 1.76                     | 0.85              |
| 31:DE:144:ARG:NH1  | 31:DE:144:ARG:HG3  | 1.91                     | 0.85              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:DS:85:VAL:C    | 41:DS:106:ARG:HG3  | 1.97                     | 0.85              |
| 27:BA:1412:A:H2'  | 27:BA:1413:G:C8    | 2.11                     | 0.85              |
| 27:BA:608:A:OP1   | 32:BF:100:THR:HG21 | 1.75                     | 0.85              |
| 42:BT:65:LYS:HZ2  | 42:BT:66:VAL:HG23  | 1.41                     | 0.85              |
| 1:CA:33:A:OP2     | 1:CA:398:C:H5'     | 1.76                     | 0.85              |
| 33:DG:37:VAL:O    | 33:DG:94:LEU:HB2   | 1.75                     | 0.85              |
| 39:DQ:45:GLN:H    | 39:DQ:45:GLN:NE2   | 1.74                     | 0.85              |
| 1:AA:854:G:H3'    | 1:AA:871:U:O4      | 1.77                     | 0.85              |
| 26:AZ:4:SER:O     | 26:AZ:5:UAL:N1     | 2.08                     | 0.85              |
| 27:BA:1111:A:O2'  | 27:BA:1112:G:H4'   | 1.75                     | 0.85              |
| 27:BA:232:G:H4'   | 27:BA:233:A:OP1    | 1.73                     | 0.85              |
| 27:BA:814:C:H41   | 38:BP:27:HIS:HD2   | 1.23                     | 0.85              |
| 27:BA:80:G:O2'    | 27:BA:81:G:H5'     | 1.76                     | 0.85              |
| 15:CO:77:ARG:HA   | 15:CO:80:ALA:HB3   | 1.59                     | 0.85              |
| 1:CA:192:U:O4'    | 20:CT:103:GLY:HA2  | 1.77                     | 0.85              |
| 27:DA:2807:G:H22  | 27:DA:2892:A:H62   | 1.24                     | 0.85              |
| 27:DA:783:A:H2'   | 27:DA:784:A:H4'    | 1.59                     | 0.85              |
| 30:DD:181:GLU:HA  | 30:DD:272:ALA:HB3  | 1.59                     | 0.85              |
| 40:DR:26:LYS:CE   | 40:DR:71:GLN:H     | 1.90                     | 0.85              |
| 41:DS:97:ARG:NH2  | 41:DS:98:VAL:HA    | 1.92                     | 0.85              |
| 48:DZ:27:MET:CE   | 48:DZ:34:ARG:HB2   | 2.06                     | 0.85              |
| 12:AL:48:ALA:O    | 12:AL:49:LEU:HD13  | 1.77                     | 0.85              |
| 10:AJ:64:GLU:HG2  | 14:AN:59:ALA:HB2   | 1.57                     | 0.85              |
| 27:BA:1591:G:H2'  | 27:BA:1592:C:C6    | 2.12                     | 0.85              |
| 27:BA:2503:A:H4'  | 27:BA:2504:U:OP1   | 1.75                     | 0.85              |
| 36:BN:133:GLN:O   | 36:BN:134:ARG:HG3  | 1.76                     | 0.85              |
| 38:BP:95:VAL:HG22 | 38:BP:125:VAL:HG12 | 1.57                     | 0.85              |
| 46:BX:80:ILE:O    | 46:BX:80:ILE:HD13  | 1.76                     | 0.85              |
| 48:BZ:81:ARG:NH2  | 48:BZ:83:GLU:HA    | 1.90                     | 0.85              |
| 24:CX:17:C:H2'    | 24:CX:17(B):U:C6   | 2.12                     | 0.85              |
| 27:DA:330:A:HO2'  | 27:DA:331:A:H8     | 1.21                     | 0.85              |
| 27:DA:796:C:H2'   | 27:DA:797:C:C6     | 2.12                     | 0.85              |
| 45:DW:84:ARG:HB2  | 45:DW:96:ILE:HG23  | 1.57                     | 0.85              |
| 27:BA:1434:A:H61  | 27:BA:1558:A:H62   | 1.18                     | 0.85              |
| 36:BN:4:TYR:CB    | 43:BU:64:ARG:HH22  | 1.88                     | 0.85              |
| 9:CI:125:TYR:CE2  | 9:CI:127:LYS:HB2   | 2.11                     | 0.85              |
| 33:BG:2:PRO:HG2   | 53:B4:51:TYR:CD2   | 2.12                     | 0.85              |
| 57:B8:50:LEU:HD12 | 57:B8:51:ALA:N     | 1.91                     | 0.85              |
| 27:BA:1006:C:H1'  | 36:BN:106:MET:HG2  | 1.56                     | 0.85              |
| 27:BA:1431:U:H2'  | 27:BA:1432:C:C6    | 2.12                     | 0.85              |
| 27:BA:363(B):G:N3 | 27:BA:363(B):G:H2' | 1.92                     | 0.85              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:CT:14:LYS:HB2  | 20:CT:17:ARG:NH2   | 1.90                     | 0.85              |
| 27:DA:999:U:C2'   | 27:DA:1000:A:H5''  | 2.07                     | 0.85              |
| 27:DA:999:U:H2'   | 27:DA:1000:A:H5''  | 1.57                     | 0.85              |
| 43:DU:87:GLY:O    | 44:DV:50:PRO:HD3   | 1.77                     | 0.85              |
| 47:DY:27:VAL:HA   | 47:DY:28:LYS:NZ    | 1.90                     | 0.85              |
| 18:AR:37:VAL:HG23 | 18:AR:38:GLU:H     | 1.39                     | 0.85              |
| 27:BA:1771:C:HO2' | 27:BA:1786:A:H8    | 0.86                     | 0.85              |
| 27:BA:2809:A:N1   | 27:BA:2892:A:H1'   | 1.92                     | 0.85              |
| 27:BA:2870:C:H2'  | 27:BA:2871:C:H5'   | 1.57                     | 0.85              |
| 31:BE:33:VAL:HG13 | 31:BE:69:LYS:HE3   | 1.58                     | 0.85              |
| 34:BH:85:LYS:CD   | 34:BH:133:VAL:HB   | 2.06                     | 0.85              |
| 47:BY:39:VAL:O    | 47:BY:40:GLU:HG2   | 1.77                     | 0.85              |
| 3:CC:83:ARG:O     | 3:CC:87:LEU:HG     | 1.76                     | 0.85              |
| 16:CP:82:GLN:H    | 16:CP:82:GLN:NE2   | 1.74                     | 0.85              |
| 27:DA:1199:U:H2'  | 27:DA:1200:C:C6    | 2.11                     | 0.85              |
| 27:DA:1484:G:H3'  | 27:DA:1485:G:H5''  | 1.58                     | 0.85              |
| 27:DA:1917:U:H2'  | 27:DA:1918:A:C8    | 2.12                     | 0.85              |
| 27:DA:2383:G:H2'  | 27:DA:2384:G:C8    | 2.12                     | 0.85              |
| 27:DA:908:C:OP1   | 39:DQ:22:LYS:HB3   | 1.77                     | 0.85              |
| 6:AF:2:ARG:HD2    | 6:AF:69:GLU:HB3    | 1.58                     | 0.84              |
| 24:AX:72:A:H3'    | 24:AX:73:A:H8      | 1.41                     | 0.84              |
| 55:B6:16:CYS:O    | 55:B6:17:LYS:HB2   | 1.75                     | 0.84              |
| 55:B6:19:ARG:HG2  | 55:B6:20:ASN:H     | 1.39                     | 0.84              |
| 27:BA:1291:C:H2'  | 27:BA:1292:U:C6    | 2.12                     | 0.84              |
| 33:BG:112:PRO:O   | 33:BG:113:ARG:NH1  | 2.10                     | 0.84              |
| 27:DA:476:G:O2'   | 27:DA:477:A:H3'    | 1.75                     | 0.84              |
| 1:AA:877:C:OP1    | 8:AH:88:LYS:HE2    | 1.76                     | 0.84              |
| 13:AM:76:ALA:HA   | 13:AM:79:LYS:CG    | 2.07                     | 0.84              |
| 27:BA:1636:C:H2'  | 27:BA:1637:A:H8    | 1.40                     | 0.84              |
| 27:BA:1887:C:H2'  | 27:BA:1888:G:H5''  | 1.59                     | 0.84              |
| 27:BA:2020:A:OP1  | 43:BU:26:GLY:HA3   | 1.77                     | 0.84              |
| 33:BG:118:ARG:H   | 33:BG:181:ARG:HH21 | 1.20                     | 0.84              |
| 34:BH:43:VAL:HG21 | 34:BH:52:VAL:HG22  | 1.59                     | 0.84              |
| 40:BR:98:LEU:HB2  | 40:BR:113:LEU:HB2  | 1.58                     | 0.84              |
| 1:CA:1137:C:H4'   | 1:CA:1138:G:N2     | 1.92                     | 0.84              |
| 54:D5:4:HIS:HB2   | 54:D5:5:PRO:HD3    | 1.59                     | 0.84              |
| 27:DA:389:G:N1    | 38:DP:71:VAL:HG12  | 1.92                     | 0.84              |
| 30:DD:218:ARG:HB3 | 30:DD:219:PRO:HD2  | 1.57                     | 0.84              |
| 42:DT:23:ARG:O    | 42:DT:25:GLY:N     | 2.10                     | 0.84              |
| 1:AA:1079:G:H2'   | 1:AA:1080:A:C8     | 2.12                     | 0.84              |
| 13:AM:76:ALA:HA   | 13:AM:79:LYS:HG3   | 1.59                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BE:132:HIS:CD2  | 31:BE:135:HIS:NE2  | 2.44                     | 0.84              |
| 31:BE:141:ILE:O    | 31:BE:150:VAL:HG13 | 1.76                     | 0.84              |
| 31:BE:37:ARG:O     | 31:BE:45:THR:HA    | 1.77                     | 0.84              |
| 1:CA:1346:A:H61    | 1:CA:1374:A:H3'    | 1.42                     | 0.84              |
| 1:CA:539:A:H2'     | 1:CA:540:G:C8      | 2.12                     | 0.84              |
| 13:CM:3:ARG:HH21   | 13:CM:7:VAL:HG13   | 1.42                     | 0.84              |
| 20:CT:26:ASN:O     | 20:CT:30:LYS:HB2   | 1.77                     | 0.84              |
| 39:DQ:101:ARG:HD2  | 39:DQ:102:VAL:H    | 1.42                     | 0.84              |
| 1:AA:189(K):U:H2'  | 1:AA:189(L):G:C8   | 2.13                     | 0.84              |
| 20:AT:26:ASN:ND2   | 20:AT:26:ASN:H     | 1.76                     | 0.84              |
| 27:BA:1114:G:C3'   | 27:BA:1115:G:H5''  | 2.07                     | 0.84              |
| 27:BA:1179:C:C2'   | 27:BA:1180:C:H5''  | 2.08                     | 0.84              |
| 27:BA:1278:A:OP1   | 40:BR:36:THR:HG22  | 1.76                     | 0.84              |
| 27:BA:71:A:H8      | 27:BA:71:A:H5'     | 1.43                     | 0.84              |
| 1:CA:1125:U:O4     | 10:CJ:5:ARG:HD3    | 1.77                     | 0.84              |
| 13:CM:13:LYS:HA    | 13:CM:44:ARG:NH1   | 1.93                     | 0.84              |
| 20:CT:76:ALA:HA    | 20:CT:79:ARG:NH1   | 1.93                     | 0.84              |
| 27:DA:2572:A:C5'   | 27:DA:2574:G:H4'   | 2.07                     | 0.84              |
| 27:DA:2808:U:O2'   | 27:DA:2809:A:H5'   | 1.76                     | 0.84              |
| 36:DN:65:LYS:O     | 36:DN:69:GLN:HB2   | 1.77                     | 0.84              |
| 38:DP:144:GLU:H    | 38:DP:145:PRO:HD3  | 1.42                     | 0.84              |
| 42:DT:28:VAL:HG21  | 42:DT:46:GLU:HG3   | 1.59                     | 0.84              |
| 42:DT:99:LEU:HB2   | 42:DT:101:PHE:CE1  | 2.11                     | 0.84              |
| 48:DZ:75:LEU:HD12  | 48:DZ:80:ARG:O     | 1.75                     | 0.84              |
| 7:AG:24:THR:HA     | 7:AG:27:ILE:HD12   | 1.57                     | 0.84              |
| 27:BA:271(F):C:H2' | 27:BA:271(G):C:O4' | 1.78                     | 0.84              |
| 27:BA:28:A:H61     | 27:BA:512:G:H1'    | 1.43                     | 0.84              |
| 34:BH:92:ILE:HG22  | 34:BH:93:GLY:H     | 1.42                     | 0.84              |
| 1:CA:539:A:H2'     | 1:CA:540:G:H8      | 1.42                     | 0.84              |
| 1:CA:735:C:H2'     | 1:CA:736:C:H6      | 1.39                     | 0.84              |
| 1:CA:935:A:H2      | 1:CA:1383:C:H42    | 1.24                     | 0.84              |
| 4:CD:8:VAL:HG12    | 4:CD:21:LEU:HD13   | 1.57                     | 0.84              |
| 55:D6:18:ARG:HD2   | 55:D6:43:CYS:SG    | 2.17                     | 0.84              |
| 27:DA:2247:A:H2'   | 27:DA:2248:C:H6    | 1.42                     | 0.84              |
| 27:DA:2734:A:H62   | 27:DA:2770:G:H21   | 1.25                     | 0.84              |
| 30:DD:77:ALA:HB3   | 30:DD:117:VAL:HG22 | 1.57                     | 0.84              |
| 39:DQ:27:VAL:H     | 39:DQ:137:TYR:HD1  | 1.25                     | 0.84              |
| 42:DT:28:VAL:HG22  | 42:DT:47:GLY:N     | 1.93                     | 0.84              |
| 27:BA:2443:C:H2'   | 27:BA:2444:G:H8    | 1.41                     | 0.84              |
| 41:BS:30:ARG:HH22  | 41:BS:62:LYS:HD2   | 1.40                     | 0.84              |
| 48:BZ:138:VAL:HG12 | 48:BZ:139:ASP:H    | 1.43                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:603:U:H2'     | 1:CA:604:G:H8      | 1.42                     | 0.84              |
| 1:CA:707:C:H2'     | 1:CA:708:C:H6      | 1.42                     | 0.84              |
| 42:DT:28:VAL:O     | 42:DT:29:ARG:HB2   | 1.75                     | 0.84              |
| 1:AA:373:A:C8      | 1:AA:373:A:H5'     | 2.13                     | 0.84              |
| 5:AE:20:GLN:HE22   | 5:AE:25:ARG:CZ     | 1.90                     | 0.84              |
| 5:AE:76:ILE:HD11   | 5:AE:142:LEU:CD2   | 2.07                     | 0.84              |
| 16:AP:21:VAL:HG13  | 16:AP:33:ILE:HB    | 1.56                     | 0.84              |
| 32:BF:123:LEU:HD12 | 32:BF:124:LEU:N    | 1.93                     | 0.84              |
| 33:BG:102:PHE:HA   | 33:BG:105:LYS:NZ   | 1.93                     | 0.84              |
| 1:CA:1342:C:H2'    | 1:CA:1343:G:C8     | 2.12                     | 0.84              |
| 1:CA:975:A:H61     | 10:CJ:48:THR:HB    | 1.41                     | 0.84              |
| 55:D6:30:THR:HB    | 55:D6:31:PRO:HD2   | 1.59                     | 0.84              |
| 27:DA:154(A):C:N4  | 27:DA:172:C:H42    | 1.75                     | 0.84              |
| 32:DF:57:VAL:CG1   | 32:DF:59:TYR:HD1   | 1.89                     | 0.84              |
| 44:DV:2:PHE:CB     | 44:DV:42:GLY:HA2   | 2.06                     | 0.84              |
| 8:AH:20:TYR:HA     | 8:AH:65:TYR:HE2    | 1.43                     | 0.84              |
| 15:AO:74:ASP:OD2   | 15:AO:77:ARG:HG2   | 1.76                     | 0.84              |
| 32:BF:160:ASN:OD1  | 32:BF:163:VAL:HG23 | 1.78                     | 0.84              |
| 38:BP:47:ASP:HB3   | 38:BP:48:PRO:HA    | 1.58                     | 0.84              |
| 44:BV:62:LEU:H     | 44:BV:62:LEU:HD22  | 1.43                     | 0.84              |
| 1:CA:199:G:HO2'    | 1:CA:200:G:H8      | 1.25                     | 0.84              |
| 8:CH:68:ARG:HG2    | 8:CH:68:ARG:HH11   | 1.41                     | 0.84              |
| 27:DA:1188:U:H4'   | 44:DV:79:VAL:HG22  | 1.60                     | 0.84              |
| 27:DA:2018:G:H21   | 43:DU:34:LYS:NZ    | 1.75                     | 0.84              |
| 27:DA:704:G:H2'    | 27:DA:726:G:N2     | 1.92                     | 0.84              |
| 27:DA:740:U:H5'    | 27:DA:740:U:C6     | 2.10                     | 0.84              |
| 15:AO:6:GLU:O      | 15:AO:10:LYS:HB3   | 1.77                     | 0.84              |
| 27:BA:1114:G:H3'   | 27:BA:1115:G:H5''  | 1.57                     | 0.84              |
| 27:BA:648:G:H2'    | 27:BA:649:G:H8     | 1.43                     | 0.84              |
| 30:BD:146:GLU:HG2  | 30:BD:152:GLY:O    | 1.77                     | 0.84              |
| 44:BV:35:LEU:HB2   | 44:BV:57:VAL:HG12  | 1.57                     | 0.84              |
| 1:CA:976:G:H5'     | 1:CA:1358:U:O2'    | 1.78                     | 0.84              |
| 2:CB:178:ARG:HH22  | 8:CH:68:ARG:HH22   | 1.21                     | 0.84              |
| 12:CL:43:LYS:HG2   | 12:CL:44:LYS:N     | 1.93                     | 0.84              |
| 35:BI:82:ARG:HB2   | 35:BI:82:ARG:HH11  | 1.40                     | 0.84              |
| 43:BU:92:ARG:O     | 43:BU:94:ASN:N     | 2.10                     | 0.84              |
| 27:DA:919:G:H5'    | 28:DB:81:G:H1'     | 1.60                     | 0.84              |
| 27:BA:2312:U:OP2   | 33:BG:74:LYS:HE2   | 1.76                     | 0.83              |
| 1:CA:1003:G:C2'    | 1:CA:1004:A:H4'    | 2.07                     | 0.83              |
| 1:CA:507:C:H2'     | 1:CA:508:C:H5      | 1.41                     | 0.83              |
| 1:CA:685:G:C2      | 1:CA:686:U:H5      | 1.96                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:916:G:H2'     | 1:CA:917:G:C8      | 2.13                     | 0.83              |
| 27:DA:2482:G:H2'   | 27:DA:2483:C:C6    | 2.13                     | 0.83              |
| 27:DA:35:G:H1'     | 27:DA:454:A:C1'    | 2.08                     | 0.83              |
| 27:DA:484:C:H2'    | 27:DA:485:C:H6     | 1.42                     | 0.83              |
| 27:DA:1244:G:H4'   | 38:DP:11:GLY:HA2   | 1.60                     | 0.83              |
| 20:AT:50:GLU:HG3   | 20:AT:51:GLU:N     | 1.91                     | 0.83              |
| 27:BA:2571:C:C5'   | 27:BA:2572:A:H5''  | 2.07                     | 0.83              |
| 27:BA:34:C:O2'     | 27:BA:35:G:H5'     | 1.78                     | 0.83              |
| 29:BC:49:ILE:HD12  | 29:BC:49:ILE:H     | 1.43                     | 0.83              |
| 38:BP:16:ARG:NH1   | 38:BP:18:ARG:HG2   | 1.91                     | 0.83              |
| 6:CF:37:VAL:HA     | 6:CF:65:VAL:HG12   | 1.59                     | 0.83              |
| 20:CT:72:LEU:HD23  | 20:CT:73:HIS:N     | 1.92                     | 0.83              |
| 27:DA:1188:U:H4'   | 44:DV:79:VAL:CG2   | 2.08                     | 0.83              |
| 27:DA:1707:G:H2'   | 27:DA:1708:C:H6    | 1.44                     | 0.83              |
| 27:DA:434:U:H4'    | 27:DA:435:C:OP1    | 1.77                     | 0.83              |
| 35:DI:5:LEU:HD12   | 35:DI:5:LEU:H      | 1.43                     | 0.83              |
| 55:B6:10:LEU:HD12  | 57:B8:34:TRP:CD1   | 2.13                     | 0.83              |
| 27:BA:1332:G:N2    | 27:BA:1609:A:O2'   | 2.11                     | 0.83              |
| 27:BA:2126:A:H4'   | 27:BA:2127:G:O5'   | 1.78                     | 0.83              |
| 27:BA:272(B):G:H1  | 27:BA:366:C:H42    | 1.23                     | 0.83              |
| 30:BD:182:LEU:O    | 30:BD:271:ILE:HG12 | 1.78                     | 0.83              |
| 33:BG:128:ARG:C    | 33:BG:130:ASN:H    | 1.77                     | 0.83              |
| 48:BZ:162:LEU:HD21 | 48:BZ:166:PRO:HG3  | 1.60                     | 0.83              |
| 1:CA:1305:G:H22    | 1:CA:1331:G:H2'    | 1.42                     | 0.83              |
| 5:CE:10:MET:HA     | 5:CE:32:VAL:HG13   | 1.58                     | 0.83              |
| 55:D6:15:GLU:OE2   | 55:D6:43:CYS:SG    | 2.36                     | 0.83              |
| 27:DA:865:C:H4'    | 27:DA:866:A:OP1    | 1.78                     | 0.83              |
| 1:AA:203:U:H1'     | 1:AA:216:G:C6      | 2.13                     | 0.83              |
| 8:AH:84:ARG:HH11   | 8:AH:84:ARG:CG     | 1.91                     | 0.83              |
| 16:AP:56:ALA:O     | 16:AP:60:LEU:HG    | 1.77                     | 0.83              |
| 55:B6:20:ASN:ND2   | 55:B6:21:TYR:H     | 1.76                     | 0.83              |
| 27:BA:2123:G:H2'   | 27:BA:2124:G:C8    | 2.12                     | 0.83              |
| 27:BA:2472:G:H5'   | 27:BA:2473:U:H5''  | 1.61                     | 0.83              |
| 34:BH:23:ARG:HB3   | 34:BH:34:GLU:OE1   | 1.78                     | 0.83              |
| 38:BP:50:ARG:HB3   | 57:B8:59:LYS:HD3   | 1.59                     | 0.83              |
| 3:CC:155:GLY:O     | 3:CC:156:ARG:HB2   | 1.78                     | 0.83              |
| 3:CC:14:ILE:HG12   | 3:CC:15:THR:H      | 1.43                     | 0.83              |
| 11:CK:79:SER:HB2   | 11:CK:106:LYS:HD2  | 1.58                     | 0.83              |
| 25:CY:35:G:H2'     | 25:CY:36:A:C8      | 2.13                     | 0.83              |
| 27:DA:2199:A:H3'   | 27:DA:2200:C:H6    | 1.42                     | 0.83              |
| 31:DE:76:ARG:HG2   | 31:DE:195:LEU:HD13 | 1.60                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DP:16:ARG:HD3   | 38:DP:18:ARG:H     | 1.41                     | 0.83              |
| 1:AA:1321:C:H5'    | 1:AA:1322:C:C5'    | 2.09                     | 0.83              |
| 12:AL:15:VAL:HG23  | 12:AL:16:ARG:N     | 1.93                     | 0.83              |
| 15:AO:3:ILE:HG22   | 15:AO:38:ARG:NH1   | 1.92                     | 0.83              |
| 27:BA:2841:C:H2'   | 27:BA:2842:G:C8    | 2.14                     | 0.83              |
| 38:BP:48:PRO:HG2   | 38:BP:49:ARG:H     | 1.42                     | 0.83              |
| 1:CA:1385:G:O2'    | 1:CA:1386:G:H5'    | 1.78                     | 0.83              |
| 1:CA:868:C:H2'     | 1:CA:869:G:O4'     | 1.77                     | 0.83              |
| 11:CK:18:ARG:HB3   | 11:CK:33:THR:OG1   | 1.79                     | 0.83              |
| 30:DD:27:THR:HG21  | 30:DD:83:GLU:HG2   | 1.60                     | 0.83              |
| 33:DG:114:ILE:HG22 | 33:DG:116:ASP:H    | 1.42                     | 0.83              |
| 43:DU:97:ASP:O     | 43:DU:100:VAL:HB   | 1.77                     | 0.83              |
| 1:AA:495:A:H1'     | 1:AA:496:A:H5'     | 1.60                     | 0.83              |
| 57:D8:4:MET:O      | 57:D8:62:LEU:HD11  | 1.77                     | 0.83              |
| 29:DC:36:LYS:HD3   | 29:DC:37:PHE:H     | 1.42                     | 0.83              |
| 38:DP:7:ARG:O      | 38:DP:10:PRO:HD2   | 1.78                     | 0.83              |
| 44:DV:31:ALA:H     | 44:DV:61:VAL:HG13  | 1.44                     | 0.83              |
| 47:DY:28:LYS:HB3   | 47:DY:39:VAL:N     | 1.94                     | 0.83              |
| 48:DZ:134:GLU:O    | 48:DZ:135:PHE:HB3  | 1.78                     | 0.83              |
| 2:AB:114:ARG:NH1   | 2:AB:118:LEU:HD21  | 1.94                     | 0.83              |
| 27:BA:2090:G:H21   | 50:B1:45:ASN:HD21  | 1.21                     | 0.83              |
| 27:BA:56:A:O2'     | 27:BA:57:C:H5'     | 1.78                     | 0.83              |
| 30:BD:101:GLU:OE1  | 30:BD:103:ARG:HD3  | 1.79                     | 0.83              |
| 30:BD:43:ARG:NH1   | 30:BD:44:ASN:ND2   | 2.27                     | 0.83              |
| 42:BT:91:ARG:CB    | 42:BT:116:ALA:HA   | 2.08                     | 0.83              |
| 1:CA:754:C:H2'     | 1:CA:754:C:O2      | 1.77                     | 0.83              |
| 27:DA:1793:C:H2'   | 27:DA:1794:U:H6    | 1.44                     | 0.83              |
| 27:DA:858:U:O2     | 27:DA:2268:A:H2'   | 1.79                     | 0.83              |
| 27:DA:322:A:OP2    | 32:DF:169:ASN:HB2  | 1.79                     | 0.83              |
| 1:AA:509:A:H5'     | 4:AD:54:TYR:HD2    | 1.41                     | 0.83              |
| 7:AG:113:GLU:HG2   | 7:AG:119:ARG:HG2   | 1.58                     | 0.83              |
| 19:AS:13:ASP:HA    | 19:AS:16:LEU:HD22  | 1.60                     | 0.83              |
| 54:B5:41:PRO:HG2   | 54:B5:44:THR:HG21  | 1.59                     | 0.83              |
| 34:BH:13:LYS:HD3   | 34:BH:14:GLY:N     | 1.92                     | 0.83              |
| 2:CB:172:ILE:HD12  | 2:CB:172:ILE:N     | 1.92                     | 0.83              |
| 27:DA:1713:U:O2'   | 27:DA:1714:G:H5'   | 1.78                     | 0.83              |
| 32:DF:2:LYS:O      | 32:DF:25:PRO:HD2   | 1.79                     | 0.83              |
| 38:DP:99:LEU:HA    | 38:DP:102:ARG:HH12 | 1.44                     | 0.83              |
| 27:DA:389:G:H1     | 38:DP:71:VAL:HG12  | 1.42                     | 0.83              |
| 40:DR:66:VAL:HG12  | 40:DR:70:LEU:HD12  | 1.61                     | 0.83              |
| 1:AA:681:C:H2'     | 1:AA:682:G:C8      | 2.13                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:25:LYS:HB2   | 12:AL:30:ARG:HH12  | 1.44                     | 0.83              |
| 50:B1:19:GLN:HB3   | 50:B1:35:THR:HG23  | 1.61                     | 0.83              |
| 35:BI:77:LEU:HB3   | 35:BI:140:LEU:HD13 | 1.60                     | 0.83              |
| 2:CB:172:ILE:CD1   | 2:CB:172:ILE:H     | 1.83                     | 0.83              |
| 7:CG:49:ILE:HG23   | 7:CG:53:LYS:HD2    | 1.60                     | 0.83              |
| 18:CR:82:THR:HG22  | 18:CR:83:GLU:N     | 1.93                     | 0.83              |
| 27:DA:1158:C:O2'   | 27:DA:1159:U:H5''  | 1.77                     | 0.83              |
| 27:DA:1673:U:H2'   | 27:DA:1674:G:H5'   | 1.61                     | 0.83              |
| 27:DA:17:G:H4'     | 43:DU:25:TRP:CH2   | 2.14                     | 0.83              |
| 27:DA:1973:G:H2'   | 27:DA:1974:C:C6    | 2.13                     | 0.83              |
| 27:DA:2351:G:H2'   | 27:DA:2365:G:H22   | 1.44                     | 0.83              |
| 27:DA:2350:C:H2'   | 27:DA:2351:G:O4'   | 1.79                     | 0.83              |
| 27:DA:2732:G:H3'   | 27:DA:2733:A:C5'   | 2.08                     | 0.83              |
| 10:AJ:49:VAL:CG2   | 14:AN:41:ARG:HB2   | 2.09                     | 0.83              |
| 27:BA:1365:A:H5''  | 50:B1:41:ARG:HH22  | 1.43                     | 0.83              |
| 27:BA:1411:C:H2'   | 27:BA:1412:A:H8    | 1.41                     | 0.83              |
| 27:BA:380:U:H3     | 27:BA:394:A:H61    | 1.27                     | 0.83              |
| 27:BA:2315:G:H21   | 33:BG:128:ARG:NH1  | 1.76                     | 0.83              |
| 36:BN:15:LEU:HD12  | 36:BN:136:GLU:HG2  | 1.59                     | 0.83              |
| 37:BO:13:ASN:HD21  | 37:BO:97:ARG:N     | 1.77                     | 0.83              |
| 36:BN:2:LYS:HZ1    | 43:BU:95:LEU:HG    | 1.42                     | 0.83              |
| 1:CA:99:U:H2'      | 1:CA:100:C:C6      | 2.13                     | 0.83              |
| 50:D1:67:ILE:N     | 50:D1:68:PRO:HD2   | 1.93                     | 0.83              |
| 27:DA:93:G:H2'     | 27:DA:94:C:O4'     | 1.76                     | 0.83              |
| 29:DC:50:ASP:HB2   | 29:DC:54:SER:O     | 1.78                     | 0.83              |
| 32:DF:167:ALA:HB1  | 32:DF:173:VAL:HG11 | 1.59                     | 0.83              |
| 38:DP:59:LEU:HA    | 38:DP:61:ARG:NH1   | 1.92                     | 0.83              |
| 42:DT:83:ILE:HG13  | 42:DT:84:GLN:H     | 1.42                     | 0.83              |
| 1:AA:1182:G:H4'    | 1:AA:1183:A:O5'    | 1.79                     | 0.82              |
| 10:AJ:51:ARG:HG2   | 14:AN:45:ARG:HH12  | 1.42                     | 0.82              |
| 27:BA:28:A:N6      | 27:BA:512:G:H1'    | 1.94                     | 0.82              |
| 27:BA:828:U:H4'    | 27:BA:831:G:N1     | 1.94                     | 0.82              |
| 1:CA:142:G:H2'     | 1:CA:143:A:C8      | 2.13                     | 0.82              |
| 1:CA:1504:G:H4'    | 1:CA:1505:G:H5'    | 1.60                     | 0.82              |
| 27:DA:1862:G:H1    | 27:DA:1880:C:H42   | 1.26                     | 0.82              |
| 27:DA:333:G:H2'    | 27:DA:334:C:C6     | 2.14                     | 0.82              |
| 32:DF:132:VAL:HG22 | 32:DF:133:ASN:H    | 1.43                     | 0.82              |
| 33:DG:28:VAL:C     | 33:DG:30:GLU:H     | 1.81                     | 0.82              |
| 46:DX:57:LEU:HD21  | 46:DX:78:LYS:HD3   | 1.61                     | 0.82              |
| 3:AC:52:LEU:HD23   | 3:AC:52:LEU:N      | 1.94                     | 0.82              |
| 58:B9:13:LYS:HD3   | 58:B9:28:GLU:HG2   | 1.61                     | 0.82              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 38:BP:23:PRO:HB2    | 38:BP:33:ARG:CD    | 2.08                     | 0.82              |
| 1:CA:817:C:H1'      | 1:CA:819:A:H5'     | 1.59                     | 0.82              |
| 2:CB:163:PHE:HA     | 2:CB:185:ILE:O     | 1.79                     | 0.82              |
| 49:D0:23:VAL:HG13   | 49:D0:38:VAL:HG22  | 1.59                     | 0.82              |
| 27:DA:1461:G:H2'    | 27:DA:1462:C:C6    | 2.13                     | 0.82              |
| 27:DA:2784:C:H1'    | 31:DE:37:ARG:NH1   | 1.94                     | 0.82              |
| 43:DU:92:ARG:HD2    | 44:DV:11:GLN:CD    | 1.99                     | 0.82              |
| 44:DV:61:VAL:HA     | 44:DV:94:LEU:HD23  | 1.61                     | 0.82              |
| 47:DY:28:LYS:HB2    | 47:DY:38:ILE:N     | 1.93                     | 0.82              |
| 1:AA:1085:U:H4'     | 1:AA:1086:U:OP2    | 1.79                     | 0.82              |
| 16:AP:82:GLN:HE21   | 16:AP:83:GLU:N     | 1.76                     | 0.82              |
| 27:BA:1860:G:H1     | 27:BA:1882:C:H42   | 1.26                     | 0.82              |
| 27:BA:2283:C:C2'    | 27:BA:2284:C:H5'   | 2.07                     | 0.82              |
| 28:BB:7:G:H3'       | 28:BB:8:U:H5''     | 1.61                     | 0.82              |
| 30:BD:243:GLY:O     | 30:BD:244:ARG:HB3  | 1.77                     | 0.82              |
| 41:BS:85:VAL:N      | 41:BS:106:ARG:HB2  | 1.93                     | 0.82              |
| 42:BT:28:VAL:HG22   | 42:BT:46:GLU:CA    | 2.09                     | 0.82              |
| 1:CA:132:C:O2       | 1:CA:230:G:N2      | 2.13                     | 0.82              |
| 1:CA:458:C:H2'      | 1:CA:460:G:H8      | 1.41                     | 0.82              |
| 1:CA:578:C:H42      | 1:CA:763:G:H1      | 1.25                     | 0.82              |
| 1:CA:979:C:C3'      | 1:CA:980:C:H5''    | 2.09                     | 0.82              |
| 27:DA:1503:U:H2'    | 27:DA:1504:C:H6    | 1.44                     | 0.82              |
| 27:DA:2801(A):A:H4' | 27:DA:2802:G:H5'   | 1.61                     | 0.82              |
| 27:DA:865:C:H2'     | 27:DA:865:C:O2     | 1.79                     | 0.82              |
| 27:DA:956:G:N2      | 27:DA:959:A:H3'    | 1.94                     | 0.82              |
| 31:DE:73:GLU:HG3    | 31:DE:74:PRO:HD2   | 1.60                     | 0.82              |
| 39:DQ:44:ALA:HB3    | 39:DQ:45:GLN:NE2   | 1.94                     | 0.82              |
| 43:DU:31:SER:HB3    | 43:DU:34:LYS:HB2   | 1.59                     | 0.82              |
| 9:AI:46:ALA:O       | 9:AI:47:LEU:HD12   | 1.79                     | 0.82              |
| 1:AA:130:A:C8       | 17:AQ:63:ARG:HG3   | 2.14                     | 0.82              |
| 56:B7:8:ASN:ND2     | 56:B7:11:LYS:H     | 1.77                     | 0.82              |
| 27:BA:639:U:H2'     | 27:BA:640:C:C6     | 2.15                     | 0.82              |
| 34:BH:148:ILE:O     | 34:BH:151:ILE:HG12 | 1.78                     | 0.82              |
| 11:CK:84:VAL:HG23   | 11:CK:110:ASP:OD1  | 1.78                     | 0.82              |
| 15:CO:12:ILE:O      | 15:CO:14:GLU:N     | 2.12                     | 0.82              |
| 27:DA:482:A:N6      | 27:DA:506:G:H2'    | 1.95                     | 0.82              |
| 2:AB:167:PRO:HG2    | 2:AB:192:SER:OG    | 1.79                     | 0.82              |
| 11:AK:32:ILE:CD1    | 11:AK:72:ALA:HB2   | 2.10                     | 0.82              |
| 27:BA:572:A:C8      | 27:BA:572:A:H5'    | 2.15                     | 0.82              |
| 27:BA:897:C:O2      | 27:BA:897:C:H2'    | 1.79                     | 0.82              |
| 37:BO:93:PRO:HG3    | 37:BO:114:ILE:HD11 | 1.61                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1250:A:H4'    | 9:CI:68:GLY:N      | 1.94                     | 0.82              |
| 1:CA:280:C:O2      | 17:CQ:38:ARG:HG3   | 1.80                     | 0.82              |
| 27:DA:271(S):G:H2' | 27:DA:271(T):C:C5' | 2.08                     | 0.82              |
| 27:DA:310:A:OP1    | 47:DY:17:SER:O     | 1.97                     | 0.82              |
| 33:DG:101:ILE:HD13 | 33:DG:102:PHE:N    | 1.94                     | 0.82              |
| 40:DR:4:LEU:HD21   | 40:DR:8:ARG:NH2    | 1.94                     | 0.82              |
| 41:DS:97:ARG:HH12  | 41:DS:99:LYS:HG2   | 1.45                     | 0.82              |
| 1:AA:443:C:H2'     | 1:AA:444:C:C6      | 2.14                     | 0.82              |
| 55:B6:41:PRO:HD3   | 55:B6:46:HIS:CA    | 2.10                     | 0.82              |
| 27:BA:2197:U:O2'   | 27:BA:2198:A:H2'   | 1.80                     | 0.82              |
| 27:BA:637:A:H4'    | 27:BA:638:G:O5'    | 1.78                     | 0.82              |
| 32:BF:41:LEU:HD11  | 32:BF:184:TYR:HE1  | 1.43                     | 0.82              |
| 27:BA:906:G:H5'    | 39:BQ:26:TYR:OH    | 1.80                     | 0.82              |
| 1:CA:1163:C:H2'    | 1:CA:1164:G:H8     | 1.45                     | 0.82              |
| 6:CF:89:MET:SD     | 18:CR:76:LEU:HD21  | 2.19                     | 0.82              |
| 8:CH:104:ARG:HB3   | 8:CH:108:GLY:H     | 1.45                     | 0.82              |
| 52:D3:59:VAL:HG12  | 52:D3:60:GLU:N     | 1.94                     | 0.82              |
| 1:AA:580:U:H2'     | 1:AA:581:G:O4'     | 1.78                     | 0.82              |
| 16:AP:82:GLN:NE2   | 16:AP:83:GLU:H     | 1.76                     | 0.82              |
| 27:BA:1607:C:H4'   | 27:BA:1608:A:O5'   | 1.80                     | 0.82              |
| 27:BA:2728:U:O2'   | 27:BA:2729:G:H5'   | 1.79                     | 0.82              |
| 27:BA:594:U:H2'    | 27:BA:595:C:C6     | 2.15                     | 0.82              |
| 30:BD:89:SER:HB2   | 30:BD:201:HIS:HD2  | 1.41                     | 0.82              |
| 38:BP:23:PRO:HD2   | 38:BP:33:ARG:HE    | 1.42                     | 0.82              |
| 27:BA:1598:C:H5'   | 46:BX:36:LYS:HB2   | 1.61                     | 0.82              |
| 1:CA:1258:G:H2'    | 1:CA:1259:C:H6     | 1.45                     | 0.82              |
| 8:CH:111:ILE:HG22  | 8:CH:112:LEU:H     | 1.44                     | 0.82              |
| 27:DA:2126:A:C6    | 27:DA:2163:C:H4'   | 2.14                     | 0.82              |
| 27:DA:2475:C:N4    | 27:DA:2529:G:H22   | 1.74                     | 0.82              |
| 27:DA:2815:C:H2'   | 27:DA:2816:C:C6    | 2.14                     | 0.82              |
| 38:DP:18:ARG:HB3   | 38:DP:18:ARG:NH1   | 1.95                     | 0.82              |
| 1:AA:495:A:H4'     | 1:AA:496:A:H5''    | 1.62                     | 0.82              |
| 55:B6:9:LEU:O      | 55:B6:9:LEU:HD23   | 1.79                     | 0.82              |
| 27:BA:154(A):C:H41 | 27:BA:172:C:H42    | 1.25                     | 0.82              |
| 27:DA:628:G:H2'    | 27:DA:629:G:C8     | 2.14                     | 0.82              |
| 27:DA:857:C:H5'    | 49:D0:77:ARG:HH12  | 1.45                     | 0.82              |
| 1:AA:979:C:H3'     | 1:AA:980:C:H5''    | 1.61                     | 0.82              |
| 2:AB:151:GLY:O     | 2:AB:152:PHE:HB2   | 1.78                     | 0.82              |
| 10:AJ:4:ILE:HG12   | 10:AJ:100:THR:CG2  | 2.10                     | 0.82              |
| 27:BA:2391:G:OP1   | 57:B8:32:LEU:HD12  | 1.79                     | 0.82              |
| 27:BA:402:A:O2'    | 27:BA:403:U:H5'    | 1.78                     | 0.82              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:BD:25:THR:O      | 30:BD:27:THR:HG22  | 1.79                     | 0.82              |
| 1:CA:458:C:H2'      | 1:CA:460:G:C8      | 2.14                     | 0.82              |
| 5:CE:91:LEU:HG      | 5:CE:120:THR:CG2   | 2.09                     | 0.82              |
| 11:CK:32:ILE:CD1    | 11:CK:41:THR:HG22  | 2.07                     | 0.82              |
| 27:DA:512:G:OP1     | 27:DA:1235:G:H5'   | 1.80                     | 0.82              |
| 27:DA:762:U:H4'     | 27:DA:763:G:O5'    | 1.78                     | 0.82              |
| 30:DD:118:VAL:CG2   | 30:DD:119:ALA:H    | 1.91                     | 0.82              |
| 1:AA:250:A:H4'      | 1:AA:251:G:O5'     | 1.80                     | 0.82              |
| 13:AM:90:LEU:O      | 13:AM:92:HIS:N     | 2.12                     | 0.82              |
| 27:BA:96:G:H4'      | 51:B2:48:HIS:CD2   | 2.15                     | 0.82              |
| 27:BA:992:C:O2'     | 27:BA:993:G:H5'    | 1.78                     | 0.82              |
| 29:BC:42:GLU:H      | 29:BC:213:TYR:H    | 1.27                     | 0.82              |
| 30:BD:68:LYS:NZ     | 30:BD:70:TRP:HE1   | 1.78                     | 0.82              |
| 33:BG:101:ILE:HG12  | 33:BG:105:LYS:HE3  | 1.59                     | 0.82              |
| 41:BS:86:ALA:N      | 41:BS:106:ARG:HG3  | 1.94                     | 0.82              |
| 47:BY:66:PRO:O      | 47:BY:67:LEU:HB3   | 1.80                     | 0.82              |
| 9:CI:24:GLY:HA2     | 9:CI:59:PHE:O      | 1.80                     | 0.82              |
| 13:CM:69:GLU:OE1    | 13:CM:69:GLU:HA    | 1.80                     | 0.82              |
| 14:CN:24:CYS:SG     | 14:CN:40:CYS:HB3   | 2.20                     | 0.82              |
| 27:DA:1493:C:H4'    | 27:DA:1494:A:OP1   | 1.78                     | 0.82              |
| 27:DA:1791:A:N6     | 27:DA:1828:G:O2'   | 2.12                     | 0.82              |
| 30:DD:24:ILE:CG1    | 30:DD:25:THR:H     | 1.84                     | 0.82              |
| 27:DA:2052:G:H4'    | 31:DE:143:ASN:O    | 1.80                     | 0.82              |
| 38:DP:23:PRO:HB2    | 38:DP:33:ARG:HD2   | 1.61                     | 0.82              |
| 8:AH:132:GLU:HG2    | 8:AH:134:ILE:HD13  | 1.60                     | 0.81              |
| 27:BA:1509(A):A:H2' | 27:BA:1509(B):A:H8 | 1.42                     | 0.81              |
| 1:CA:664:G:H22      | 1:CA:741:G:H1      | 1.24                     | 0.81              |
| 1:CA:918:A:H2'      | 1:CA:919:A:H8      | 1.44                     | 0.81              |
| 55:D6:32:ASN:O      | 55:D6:33:LYS:HB2   | 1.79                     | 0.81              |
| 27:DA:1668:A:H5'    | 27:DA:1669:A:N7    | 1.94                     | 0.81              |
| 27:DA:628:G:H2'     | 27:DA:629:G:H8     | 1.43                     | 0.81              |
| 36:DN:28:THR:HG23   | 36:DN:29:LYS:H     | 1.44                     | 0.81              |
| 44:DV:66:ARG:NH2    | 44:DV:88:ARG:HD3   | 1.94                     | 0.81              |
| 1:AA:681:C:H2'      | 1:AA:682:G:H8      | 1.43                     | 0.81              |
| 50:B1:37:ILE:HG22   | 50:B1:38:SER:N     | 1.94                     | 0.81              |
| 55:B6:11:LEU:HD11   | 55:B6:51:GLU:HG2   | 1.61                     | 0.81              |
| 30:BD:24:ILE:HG13   | 30:BD:25:THR:H     | 1.43                     | 0.81              |
| 35:BI:123:LEU:HD23  | 35:BI:142:VAL:HG12 | 1.62                     | 0.81              |
| 42:BT:54:ARG:HA     | 42:BT:59:THR:HB    | 1.60                     | 0.81              |
| 17:CQ:26:GLN:HB3    | 17:CQ:37:LYS:HG2   | 1.62                     | 0.81              |
| 52:D3:7:LYS:O       | 52:D3:54:VAL:HG13  | 1.78                     | 0.81              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 27:DA:1019:U:H3    | 27:DA:1142(A):A:H62 | 1.24                     | 0.81              |
| 27:DA:1885:A:H2'   | 27:DA:1886:C:O4'    | 1.78                     | 0.81              |
| 32:DF:32:LEU:HD23  | 32:DF:32:LEU:O      | 1.80                     | 0.81              |
| 1:AA:1380:U:H4'    | 1:AA:1381:U:O5'     | 1.81                     | 0.81              |
| 1:AA:598:U:H2'     | 1:AA:599:C:H6       | 1.43                     | 0.81              |
| 1:AA:627:G:H2'     | 1:AA:628:G:H8       | 1.43                     | 0.81              |
| 2:AB:14:GLY:O      | 2:AB:15:VAL:HG13    | 1.80                     | 0.81              |
| 24:AX:4:G:H2'      | 24:AX:5:G:C8        | 2.15                     | 0.81              |
| 33:BG:11:TYR:HA    | 33:BG:15:VAL:HB     | 1.60                     | 0.81              |
| 1:CA:1305:G:H22    | 1:CA:1331:G:C2'     | 1.92                     | 0.81              |
| 1:CA:148:G:H1      | 1:CA:174:C:H42      | 1.28                     | 0.81              |
| 1:CA:284:G:H2'     | 1:CA:285:G:H8       | 1.44                     | 0.81              |
| 3:CC:47:LEU:HD21   | 3:CC:68:VAL:HG11    | 1.61                     | 0.81              |
| 27:DA:1884:A:C2'   | 27:DA:1885:A:H5''   | 2.11                     | 0.81              |
| 27:DA:2562:U:O2    | 27:DA:2562:U:H2'    | 1.78                     | 0.81              |
| 27:DA:438:G:H2'    | 27:DA:440:G:C8      | 2.14                     | 0.81              |
| 29:DC:212:VAL:O    | 29:DC:218:MET:HA    | 1.78                     | 0.81              |
| 30:DD:112:GLN:H    | 30:DD:115:GLN:NE2   | 1.78                     | 0.81              |
| 34:DH:159:GLU:HG3  | 34:DH:160:LYS:HG3   | 1.59                     | 0.81              |
| 15:AO:62:GLN:HA    | 15:AO:65:ARG:HH11   | 1.45                     | 0.81              |
| 27:BA:1603:A:H5'   | 27:BA:1603:A:H8     | 1.46                     | 0.81              |
| 36:BN:67:LEU:O     | 36:BN:68:GLU:HG2    | 1.79                     | 0.81              |
| 41:BS:46:VAL:HG12  | 41:BS:47:THR:N      | 1.95                     | 0.81              |
| 43:BU:27:LEU:N     | 43:BU:27:LEU:HD23   | 1.96                     | 0.81              |
| 43:BU:92:ARG:NE    | 44:BV:11:GLN:HB2    | 1.94                     | 0.81              |
| 1:CA:165:C:H2'     | 1:CA:166:G:H8       | 1.43                     | 0.81              |
| 56:D7:8:ASN:HD21   | 56:D7:11:LYS:H      | 1.28                     | 0.81              |
| 27:DA:1983:C:H4'   | 27:DA:2606:C:H4'    | 1.63                     | 0.81              |
| 27:DA:525:U:O2'    | 27:DA:526:A:H5'     | 1.78                     | 0.81              |
| 27:DA:644:A:H4'    | 27:DA:645:C:C5      | 2.15                     | 0.81              |
| 31:DE:111:ARG:HD2  | 31:DE:160:TYR:CE1   | 2.14                     | 0.81              |
| 38:DP:123:LEU:HD12 | 38:DP:125:VAL:HG12  | 1.63                     | 0.81              |
| 39:DQ:32:TYR:HE2   | 39:DQ:133:ARG:HG2   | 1.45                     | 0.81              |
| 5:AE:101:ILE:N     | 5:AE:101:ILE:HD13   | 1.95                     | 0.81              |
| 15:AO:82:ILE:HD11  | 15:AO:87:ILE:H      | 1.44                     | 0.81              |
| 23:AW:6:U:C3'      | 23:AW:7:A:H5''      | 2.09                     | 0.81              |
| 27:BA:1484:G:C3'   | 27:BA:1485:G:H5''   | 2.09                     | 0.81              |
| 27:BA:389:G:H1     | 38:BP:71:VAL:HG12   | 1.45                     | 0.81              |
| 29:BC:41:VAL:O     | 29:BC:178:ALA:HB3   | 1.80                     | 0.81              |
| 2:CB:187:LEU:HD13  | 2:CB:187:LEU:O      | 1.81                     | 0.81              |
| 5:CE:76:ILE:HD11   | 5:CE:142:LEU:HD11   | 1.60                     | 0.81              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:1794:U:H2'  | 27:DA:1795:C:C6    | 2.15                     | 0.81              |
| 27:DA:941:A:H4'   | 38:DP:35:HIS:CE1   | 2.14                     | 0.81              |
| 36:DN:55:VAL:HG22 | 36:DN:126:PRO:HA   | 1.62                     | 0.81              |
| 39:DQ:66:ILE:O    | 39:DQ:66:ILE:HG13  | 1.80                     | 0.81              |
| 39:DQ:20:ALA:O    | 39:DQ:98:LYS:HB3   | 1.80                     | 0.81              |
| 4:AD:8:VAL:O      | 4:AD:10:ARG:N      | 2.13                     | 0.81              |
| 1:CA:17:U:H2'     | 1:CA:18:C:C6       | 2.16                     | 0.81              |
| 24:CX:51:C:H2'    | 24:CX:52:G:H8      | 1.44                     | 0.81              |
| 27:DA:184:C:H2'   | 27:DA:185:U:C6     | 2.14                     | 0.81              |
| 27:DA:1968:G:O2'  | 27:DA:1969:A:H5''  | 1.81                     | 0.81              |
| 27:BA:1564:C:O2'  | 27:BA:1565:C:H5'   | 1.81                     | 0.81              |
| 30:BD:65:ILE:HG12 | 30:BD:104:TYR:O    | 1.80                     | 0.81              |
| 35:BI:3:VAL:HA    | 35:BI:39:ALA:HB2   | 1.61                     | 0.81              |
| 36:BN:62:VAL:CG2  | 36:BN:66:LYS:HB2   | 2.11                     | 0.81              |
| 39:BQ:63:LYS:HZ3  | 48:BZ:174:VAL:HG11 | 1.44                     | 0.81              |
| 10:CJ:6:ILE:HG13  | 10:CJ:72:VAL:O     | 1.80                     | 0.81              |
| 27:DA:1278:A:H5'' | 40:DR:36:THR:HG22  | 1.62                     | 0.81              |
| 27:DA:1485:G:H2'  | 27:DA:1486:A:C8    | 2.16                     | 0.81              |
| 27:DA:1512:U:H2'  | 27:DA:1513:C:H6    | 1.44                     | 0.81              |
| 27:DA:873:G:N2    | 27:DA:905:U:H1'    | 1.96                     | 0.81              |
| 27:DA:917:A:H2'   | 27:DA:918:A:H8     | 1.46                     | 0.81              |
| 28:DB:87:G:C3'    | 28:DB:88:C:H5''    | 2.11                     | 0.81              |
| 36:DN:67:LEU:O    | 36:DN:68:GLU:HB2   | 1.77                     | 0.81              |
| 39:DQ:34:LEU:HD13 | 39:DQ:118:LEU:HD22 | 1.62                     | 0.81              |
| 39:DQ:56:ARG:HA   | 39:DQ:56:ARG:CZ    | 2.11                     | 0.81              |
| 48:DZ:6:ALA:HB3   | 48:DZ:58:LEU:HB3   | 1.63                     | 0.81              |
| 57:B8:33:ASN:ND2  | 57:B8:33:ASN:N     | 2.29                     | 0.81              |
| 57:B8:49:VAL:HG23 | 57:B8:53:PRO:HB3   | 1.63                     | 0.81              |
| 27:BA:2138:C:H2'  | 27:BA:2139:C:C6    | 2.15                     | 0.81              |
| 27:BA:2476:A:C2'  | 27:BA:2477:C:H5''  | 2.11                     | 0.81              |
| 27:BA:754:C:H2'   | 27:BA:755:C:C6     | 2.15                     | 0.81              |
| 38:BP:125:VAL:O   | 38:BP:145:PRO:HD2  | 1.80                     | 0.81              |
| 43:BU:26:GLY:C    | 43:BU:28:ARG:H     | 1.83                     | 0.81              |
| 1:CA:52:G:H2'     | 1:CA:53:A:H8       | 1.46                     | 0.81              |
| 1:CA:980:C:H1'    | 14:CN:19:ARG:HG2   | 1.63                     | 0.81              |
| 2:CB:11:LEU:HB3   | 2:CB:213:LEU:HD11  | 1.59                     | 0.81              |
| 27:DA:1485:G:H2'  | 27:DA:1486:A:H8    | 1.45                     | 0.81              |
| 27:DA:2199:A:H5'' | 27:DA:2200:C:H5    | 1.46                     | 0.81              |
| 27:DA:221:A:H4'   | 27:DA:222:A:O5'    | 1.81                     | 0.81              |
| 27:DA:227:A:H61   | 27:DA:410:G:H21    | 1.29                     | 0.81              |
| 40:DR:18:LEU:HD11 | 40:DR:22:ARG:CZ    | 2.11                     | 0.81              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:AL:38:ARG:HH12   | 12:AL:54:LYS:HZ2   | 1.28                     | 0.81              |
| 27:BA:2462:U:H3     | 27:BA:2488:A:H61   | 1.24                     | 0.81              |
| 39:BQ:26:TYR:CD1    | 39:BQ:28:ALA:HB2   | 2.16                     | 0.81              |
| 47:BY:31:LEU:CB     | 47:BY:32:PRO:HA    | 2.09                     | 0.81              |
| 6:CF:69:GLU:O       | 6:CF:72:VAL:HG12   | 1.81                     | 0.81              |
| 12:CL:22:PRO:O      | 12:CL:24:LEU:HD13  | 1.80                     | 0.81              |
| 27:DA:1221(A):C:H42 | 27:DA:1228:G:H1    | 1.29                     | 0.81              |
| 27:DA:2443:C:H2'    | 27:DA:2444:G:H8    | 1.43                     | 0.81              |
| 33:DG:112:PRO:O     | 33:DG:113:ARG:NH1  | 2.13                     | 0.81              |
| 27:DA:587:C:H3'     | 38:DP:33:ARG:NH2   | 1.95                     | 0.81              |
| 1:AA:487:A:H2'      | 1:AA:488:C:O4'     | 1.81                     | 0.81              |
| 3:AC:173:VAL:O      | 3:AC:175:LEU:HD12  | 1.78                     | 0.81              |
| 12:AL:20:LYS:O      | 12:AL:21:VAL:HG23  | 1.81                     | 0.81              |
| 27:BA:2290:G:H5'    | 27:BA:2290:G:H8    | 1.43                     | 0.81              |
| 1:CA:1398:A:H5''    | 1:CA:1398:A:C8     | 2.15                     | 0.81              |
| 1:CA:1513:A:H2'     | 1:CA:1514:C:C6     | 2.15                     | 0.81              |
| 1:CA:939:G:H5''     | 7:CG:102:ARG:HH22  | 1.45                     | 0.81              |
| 27:DA:1747(A):G:C2' | 27:DA:1748:G:H5''  | 2.11                     | 0.81              |
| 32:DF:141:ALA:O     | 32:DF:144:LYS:HB3  | 1.81                     | 0.81              |
| 1:AA:1116:C:H2'     | 1:AA:1117:G:H5'    | 1.63                     | 0.81              |
| 1:AA:1513:A:H2'     | 1:AA:1514:C:C6     | 2.15                     | 0.81              |
| 56:B7:8:ASN:HD21    | 56:B7:11:LYS:H     | 1.29                     | 0.81              |
| 27:BA:1782:C:H1'    | 27:BA:2609:U:H5''  | 1.61                     | 0.81              |
| 33:BG:6:ALA:HB3     | 33:BG:104:GLU:OE1  | 1.80                     | 0.81              |
| 42:BT:28:VAL:HG22   | 42:BT:47:GLY:N     | 1.96                     | 0.81              |
| 1:CA:924:C:H2'      | 1:CA:925:G:C8      | 2.16                     | 0.81              |
| 6:CF:91:VAL:HG11    | 18:CR:72:ARG:HH12  | 1.44                     | 0.81              |
| 50:D1:52:ARG:HG3    | 50:D1:53:VAL:N     | 1.96                     | 0.81              |
| 27:DA:1826:G:H2'    | 27:DA:1827:C:H6    | 1.42                     | 0.81              |
| 30:DD:133:LEU:CD1   | 30:DD:175:LEU:HD11 | 2.10                     | 0.81              |
| 33:DG:105:LYS:CE    | 53:D4:52:SER:HB3   | 2.09                     | 0.81              |
| 1:AA:1123:A:H4'     | 10:AJ:36:GLY:HA3   | 1.63                     | 0.80              |
| 19:AS:31:ILE:HG23   | 19:AS:49:ILE:HG23  | 1.62                     | 0.80              |
| 52:B3:59:VAL:HG12   | 52:B3:60:GLU:N     | 1.96                     | 0.80              |
| 27:BA:90:U:H2'      | 27:BA:90:U:O2      | 1.79                     | 0.80              |
| 1:CA:373:A:H2'      | 1:CA:374:A:C8      | 2.16                     | 0.80              |
| 51:D2:2:LYS:O       | 51:D2:6:VAL:HG23   | 1.80                     | 0.80              |
| 27:DA:1473:G:C2'    | 27:DA:1474:C:H5'   | 2.11                     | 0.80              |
| 27:DA:2152:G:H2'    | 27:DA:2153:G:H8    | 1.43                     | 0.80              |
| 27:DA:754:C:H2'     | 27:DA:755:C:C6     | 2.15                     | 0.80              |
| 38:DP:112:LEU:H     | 38:DP:128:HIS:CD2  | 1.99                     | 0.80              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:DT:57:PHE:CD2  | 42:DT:58:ASN:N     | 2.47                     | 0.80              |
| 1:AA:322:C:H2'    | 1:AA:323:U:H6      | 1.44                     | 0.80              |
| 1:AA:37:U:O2'     | 1:AA:500:G:H4'     | 1.81                     | 0.80              |
| 2:AB:178:ARG:HH12 | 2:AB:196:LEU:CB    | 1.94                     | 0.80              |
| 2:AB:44:LEU:HD12  | 2:AB:44:LEU:H      | 1.45                     | 0.80              |
| 2:AB:49:GLU:O     | 2:AB:52:GLU:HB3    | 1.81                     | 0.80              |
| 12:AL:15:VAL:HG23 | 12:AL:16:ARG:H     | 1.46                     | 0.80              |
| 57:B8:52:LYS:N    | 57:B8:53:PRO:HD2   | 1.96                     | 0.80              |
| 27:BA:1359:A:H62  | 27:BA:1372:U:H3    | 1.28                     | 0.80              |
| 30:BD:33:LEU:HD12 | 30:BD:33:LEU:H     | 1.45                     | 0.80              |
| 1:CA:742:G:C5'    | 15:CO:58:MET:HE1   | 2.11                     | 0.80              |
| 27:DA:2752:C:H2'  | 27:DA:2753:A:H8    | 1.45                     | 0.80              |
| 27:DA:660:G:H2'   | 27:DA:661:C:O4'    | 1.80                     | 0.80              |
| 30:DD:65:ILE:H    | 30:DD:65:ILE:HD13  | 1.46                     | 0.80              |
| 32:DF:2:LYS:HD3   | 32:DF:2:LYS:N      | 1.96                     | 0.80              |
| 36:DN:16:ILE:O    | 36:DN:54:VAL:HA    | 1.80                     | 0.80              |
| 15:AO:36:ILE:HG23 | 15:AO:56:LEU:HD11  | 1.64                     | 0.80              |
| 27:BA:1019:U:HO2' | 27:BA:1021:A:H2    | 0.83                     | 0.80              |
| 27:BA:2056:G:N2   | 54:B5:4:HIS:O      | 2.13                     | 0.80              |
| 37:BO:63:VAL:HG12 | 37:BO:106:LEU:HD11 | 1.61                     | 0.80              |
| 40:BR:41:ALA:O    | 40:BR:44:LEU:N     | 2.15                     | 0.80              |
| 1:CA:194:C:H2'    | 1:CA:195:A:H5''    | 1.61                     | 0.80              |
| 1:CA:677:U:H3     | 1:CA:714:G:H22     | 1.29                     | 0.80              |
| 1:CA:680:C:H2'    | 1:CA:681:C:C6      | 2.15                     | 0.80              |
| 27:DA:581:C:H2'   | 27:DA:582:G:H8     | 1.46                     | 0.80              |
| 27:DA:665:C:H2'   | 27:DA:666:G:H8     | 1.44                     | 0.80              |
| 29:DC:51:PRO:HG3  | 29:DC:204:ALA:HB2  | 1.62                     | 0.80              |
| 29:DC:83:ILE:HA   | 29:DC:94:VAL:HG21  | 1.61                     | 0.80              |
| 30:DD:168:ARG:H   | 30:DD:168:ARG:HD3  | 1.44                     | 0.80              |
| 31:DE:51:PHE:O    | 31:DE:74:PRO:HB2   | 1.80                     | 0.80              |
| 31:DE:93:VAL:C    | 31:DE:95:ILE:H     | 1.85                     | 0.80              |
| 35:DI:133:HIS:CB  | 35:DI:134:PRO:HD3  | 2.11                     | 0.80              |
| 39:DQ:45:GLN:HE21 | 39:DQ:45:GLN:N     | 1.78                     | 0.80              |
| 46:DX:25:LYS:NZ   | 46:DX:80:ILE:HD11  | 1.97                     | 0.80              |
| 1:AA:815:A:H5''   | 1:AA:817:C:H41     | 1.47                     | 0.80              |
| 16:AP:13:HIS:C    | 16:AP:15:PRO:HD3   | 2.02                     | 0.80              |
| 20:AT:71:THR:HG22 | 20:AT:72:LEU:N     | 1.95                     | 0.80              |
| 27:BA:1021:A:C8   | 27:BA:1021:A:H3'   | 2.17                     | 0.80              |
| 27:BA:1919:A:H5'' | 27:BA:1920:C:H5    | 1.47                     | 0.80              |
| 30:BD:165:ILE:HA  | 30:BD:175:LEU:HD23 | 1.62                     | 0.80              |
| 30:BD:270:ILE:O   | 30:BD:271:ILE:HG23 | 1.81                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:BF:202:PHE:O    | 32:BF:205:ARG:HB3  | 1.82                     | 0.80              |
| 1:CA:414:A:H2'     | 1:CA:415:A:O4'     | 1.80                     | 0.80              |
| 2:CB:80:ILE:HD11   | 2:CB:212:GLN:HA    | 1.64                     | 0.80              |
| 20:CT:26:ASN:HA    | 20:CT:29:LYS:HG2   | 1.62                     | 0.80              |
| 25:CY:37:U:H3'     | 25:CY:38:U:H5''    | 1.63                     | 0.80              |
| 50:D1:69:LYS:HE2   | 50:D1:72:GLU:OE2   | 1.81                     | 0.80              |
| 33:DG:63:ILE:HA    | 33:DG:143:GLU:HG3  | 1.63                     | 0.80              |
| 36:DN:89:LYS:HB3   | 36:DN:89:LYS:HZ2   | 1.44                     | 0.80              |
| 27:DA:627:A:H62    | 38:DP:84:ASN:ND2   | 1.79                     | 0.80              |
| 46:DX:12:VAL:CG1   | 46:DX:27:THR:HG23  | 2.10                     | 0.80              |
| 27:DA:84:A:H5''    | 47:DY:9:LYS:HZ1    | 1.47                     | 0.80              |
| 1:AA:405:U:O2      | 1:AA:498:U:H2'     | 1.81                     | 0.80              |
| 5:AE:20:GLN:OE1    | 5:AE:25:ARG:HD2    | 1.82                     | 0.80              |
| 32:BF:20:LEU:HD13  | 32:BF:203:GLN:HE22 | 1.45                     | 0.80              |
| 1:CA:477:A:O2'     | 1:CA:479:C:H5'     | 1.80                     | 0.80              |
| 2:CB:233:SER:OG    | 2:CB:234:PRO:HD2   | 1.82                     | 0.80              |
| 4:CD:150:GLU:H     | 4:CD:150:GLU:CD    | 1.83                     | 0.80              |
| 27:DA:943:U:OP1    | 38:DP:38:GLN:HB3   | 1.82                     | 0.80              |
| 10:AJ:49:VAL:HG21  | 14:AN:41:ARG:HB2   | 1.63                     | 0.80              |
| 27:BA:335:C:H5''   | 47:BY:73:ARG:NH2   | 1.97                     | 0.80              |
| 28:BB:40:U:H3      | 28:BB:43:C:C5'     | 1.95                     | 0.80              |
| 30:BD:43:ARG:HH11  | 30:BD:44:ASN:CG    | 1.85                     | 0.80              |
| 33:BG:177:GLY:O    | 33:BG:179:PRO:HD3  | 1.81                     | 0.80              |
| 41:BS:85:VAL:HG23  | 41:BS:106:ARG:CB   | 2.11                     | 0.80              |
| 45:BW:90:ARG:CG    | 45:BW:90:ARG:HH11  | 1.93                     | 0.80              |
| 16:CP:71:ARG:HA    | 16:CP:74:LEU:HD12  | 1.64                     | 0.80              |
| 27:DA:1784:A:H4'   | 27:DA:1785:A:O5'   | 1.80                     | 0.80              |
| 31:DE:188:VAL:HG22 | 31:DE:189:PRO:HD2  | 1.63                     | 0.80              |
| 1:AA:233:C:H2'     | 1:AA:233:C:O2      | 1.79                     | 0.80              |
| 13:AM:65:LYS:HG3   | 13:AM:69:GLU:O     | 1.81                     | 0.80              |
| 27:BA:142:A:H8     | 27:BA:1408:C:H1'   | 1.43                     | 0.80              |
| 1:CA:1109:C:H2'    | 1:CA:1110:A:O4'    | 1.82                     | 0.80              |
| 3:CC:53:ALA:HB2    | 3:CC:115:LEU:CD2   | 2.11                     | 0.80              |
| 14:CN:41:ARG:HG3   | 14:CN:42:ILE:N     | 1.97                     | 0.80              |
| 32:DF:157:VAL:HB   | 32:DF:194:MET:HB3  | 1.63                     | 0.80              |
| 9:AI:4:TYR:HA      | 9:AI:88:TYR:CE1    | 2.15                     | 0.80              |
| 34:BH:126:PRO:O    | 34:BH:127:GLU:HB2  | 1.80                     | 0.80              |
| 35:BI:115:ALA:HB2  | 35:BI:129:THR:OG1  | 1.80                     | 0.80              |
| 41:BS:97:ARG:HE    | 41:BS:98:VAL:N     | 1.80                     | 0.80              |
| 1:CA:628:G:H2'     | 1:CA:629:G:H8      | 1.45                     | 0.80              |
| 10:CJ:51:ARG:HE    | 10:CJ:61:GLU:HB2   | 1.47                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:D0:20:ARG:CG   | 49:D0:20:ARG:HH11 | 1.95                     | 0.80              |
| 39:DQ:30:GLY:HA3  | 39:DQ:106:VAL:O   | 1.81                     | 0.80              |
| 1:AA:1002:G:N2    | 1:AA:1003:G:H1'   | 1.96                     | 0.80              |
| 1:AA:1220:G:H2'   | 1:AA:1221:G:H8    | 1.45                     | 0.80              |
| 14:AN:12:ARG:C    | 14:AN:14:PRO:HD2  | 2.01                     | 0.80              |
| 27:BA:2206:G:N2   | 27:BA:2207:G:H5'  | 1.96                     | 0.80              |
| 32:BF:135:LYS:HB3 | 32:BF:138:GLU:CG  | 2.12                     | 0.80              |
| 40:BR:33:ARG:HG3  | 40:BR:115:GLU:HB3 | 1.62                     | 0.80              |
| 43:BU:69:CYS:HB2  | 43:BU:74:LEU:HD13 | 1.64                     | 0.80              |
| 1:CA:769:G:O2'    | 1:CA:770:C:H5'    | 1.82                     | 0.80              |
| 2:CB:218:ALA:O    | 2:CB:222:ILE:HG13 | 1.82                     | 0.80              |
| 3:CC:52:LEU:HD23  | 3:CC:52:LEU:H     | 1.47                     | 0.80              |
| 8:CH:24:THR:HG22  | 8:CH:25:ASP:H     | 1.47                     | 0.80              |
| 12:CL:67:ILE:CD1  | 12:CL:74:LEU:HD12 | 2.12                     | 0.80              |
| 38:DP:65:ARG:HH11 | 57:D8:46:ARG:HH22 | 1.29                     | 0.80              |
| 27:DA:2037:G:H2'  | 27:DA:2038:G:C8   | 2.17                     | 0.80              |
| 27:DA:2692:C:O2'  | 27:DA:2693:A:H5'  | 1.82                     | 0.80              |
| 27:DA:412:A:H8    | 27:DA:412:A:H5'   | 1.47                     | 0.80              |
| 31:DE:203:LYS:HE3 | 31:DE:203:LYS:C   | 2.01                     | 0.80              |
| 36:DN:25:ARG:HG3  | 36:DN:25:ARG:HH11 | 1.47                     | 0.80              |
| 39:DQ:10:ARG:HG3  | 39:DQ:10:ARG:HH11 | 1.44                     | 0.80              |
| 4:AD:105:VAL:HG13 | 4:AD:110:PHE:HD2  | 1.48                     | 0.80              |
| 8:AH:103:VAL:HG21 | 8:AH:110:ALA:HB2  | 1.64                     | 0.80              |
| 27:BA:2047:U:H2'  | 27:BA:2048:G:H5'  | 1.64                     | 0.80              |
| 27:BA:1353:A:H4'  | 30:BD:38:LYS:HE3  | 1.63                     | 0.80              |
| 1:CA:1250:A:H5'   | 9:CI:67:GLY:HA2   | 1.62                     | 0.80              |
| 1:CA:885:G:H2'    | 1:CA:886:G:H8     | 1.47                     | 0.80              |
| 9:CI:48:GLU:N     | 9:CI:49:PRO:HD2   | 1.97                     | 0.80              |
| 30:DD:61:LEU:HB3  | 30:DD:63:ARG:HH12 | 1.42                     | 0.80              |
| 36:DN:78:TYR:HB3  | 36:DN:79:PRO:CD   | 2.09                     | 0.80              |
| 41:DS:77:ALA:HB1  | 41:DS:82:ILE:HB   | 1.64                     | 0.80              |
| 41:DS:90:GLY:C    | 41:DS:92:TYR:H    | 1.84                     | 0.80              |
| 41:DS:97:ARG:HH21 | 41:DS:98:VAL:HA   | 1.44                     | 0.80              |
| 42:DT:35:LYS:HE2  | 42:DT:41:ARG:HG3  | 1.64                     | 0.80              |
| 48:DZ:72:GLN:HG2  | 48:DZ:86:ASP:OD1  | 1.81                     | 0.80              |
| 1:AA:178:C:H2'    | 1:AA:179:A:H8     | 1.44                     | 0.79              |
| 4:AD:26:CYS:HA    | 4:AD:31:CYS:HB2   | 1.64                     | 0.79              |
| 27:BA:152:G:H1    | 27:BA:174:C:N4    | 1.77                     | 0.79              |
| 27:BA:2200:C:C6   | 27:BA:2200:C:H5'' | 2.15                     | 0.79              |
| 1:CA:1057:G:H5''  | 3:CC:154:SER:OG   | 1.82                     | 0.79              |
| 27:DA:1826:G:H2'  | 27:DA:1827:C:C6   | 2.15                     | 0.79              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:855:G:H2'   | 27:DA:856:C:C6     | 2.17                     | 0.79              |
| 28:DB:7:G:C2'     | 28:DB:8:U:H5''     | 2.12                     | 0.79              |
| 36:DN:120:LEU:CD1 | 36:DN:122:VAL:HG23 | 2.12                     | 0.79              |
| 1:AA:1199:U:H4'   | 10:AJ:54:PHE:CZ    | 2.17                     | 0.79              |
| 1:AA:1424:C:H42   | 1:AA:1476:G:H1     | 1.30                     | 0.79              |
| 1:AA:69:G:H2'     | 1:AA:70:G:C8       | 2.17                     | 0.79              |
| 1:AA:833:U:H3     | 1:AA:853:G:H1      | 1.30                     | 0.79              |
| 13:AM:17:VAL:O    | 13:AM:20:THR:HB    | 1.82                     | 0.79              |
| 17:AQ:17:LYS:CG   | 17:AQ:47:PRO:HA    | 2.05                     | 0.79              |
| 27:BA:1931:U:C6   | 27:BA:1931:U:H5'   | 2.17                     | 0.79              |
| 27:BA:2173:A:O2'  | 27:BA:2174:C:H5'   | 1.81                     | 0.79              |
| 27:BA:2355:C:H1'  | 49:B0:39:ARG:HH21  | 1.46                     | 0.79              |
| 46:BX:57:LEU:HD21 | 46:BX:78:LYS:HE2   | 1.64                     | 0.79              |
| 1:CA:1094:G:H3'   | 1:CA:1108:G:H22    | 1.47                     | 0.79              |
| 1:CA:158:G:O2'    | 1:CA:159:G:H5'     | 1.83                     | 0.79              |
| 12:CL:21:VAL:O    | 12:CL:21:VAL:HG13  | 1.80                     | 0.79              |
| 1:CA:1060:C:H5'   | 14:CN:45:ARG:NH2   | 1.98                     | 0.79              |
| 20:CT:54:LYS:HA   | 20:CT:57:ARG:NH2   | 1.97                     | 0.79              |
| 27:DA:1163:G:O2'  | 27:DA:1164:G:H5'   | 1.82                     | 0.79              |
| 27:DA:1494:A:N3   | 27:DA:1494:A:H5'   | 1.97                     | 0.79              |
| 27:DA:2784:C:O2'  | 27:DA:2785:C:H5'   | 1.83                     | 0.79              |
| 27:DA:428:A:H5'   | 27:DA:429:A:OP2    | 1.82                     | 0.79              |
| 47:DY:39:VAL:HG12 | 47:DY:40:GLU:N     | 1.96                     | 0.79              |
| 1:AA:1118:C:H2'   | 1:AA:1119:C:H6     | 1.47                     | 0.79              |
| 1:AA:60:A:H4'     | 1:AA:61:G:O5'      | 1.80                     | 0.79              |
| 4:AD:33:MET:CE    | 4:AD:37:PRO:HA     | 2.13                     | 0.79              |
| 13:AM:76:ALA:N    | 13:AM:79:LYS:HZ2   | 1.81                     | 0.79              |
| 57:B8:28:GLY:O    | 57:B8:32:LEU:HD23  | 1.81                     | 0.79              |
| 33:BG:43:LEU:HB2  | 33:BG:88:ILE:CD1   | 2.13                     | 0.79              |
| 34:BH:85:LYS:NZ   | 34:BH:133:VAL:HG11 | 1.96                     | 0.79              |
| 38:BP:23:PRO:HB2  | 38:BP:33:ARG:CG    | 2.12                     | 0.79              |
| 38:BP:59:LEU:HA   | 38:BP:61:ARG:NH2   | 1.97                     | 0.79              |
| 42:BT:122:ASP:C   | 42:BT:124:ASP:H    | 1.85                     | 0.79              |
| 44:BV:18:LEU:CD1  | 44:BV:19:LYS:H     | 1.93                     | 0.79              |
| 44:BV:57:VAL:HG23 | 44:BV:99:ILE:HG22  | 1.64                     | 0.79              |
| 52:D3:7:LYS:HG3   | 52:D3:34:GLU:HG2   | 1.62                     | 0.79              |
| 27:DA:768:G:H2'   | 27:DA:769:G:H8     | 1.47                     | 0.79              |
| 31:DE:15:PHE:CE2  | 42:DT:80:SER:HB2   | 2.16                     | 0.79              |
| 48:DZ:4:LEU:HD12  | 48:DZ:5:LYS:H      | 1.45                     | 0.79              |
| 13:AM:22:ILE:HB   | 13:AM:25:ILE:HB    | 1.64                     | 0.79              |
| 13:AM:69:GLU:HA   | 13:AM:69:GLU:OE1   | 1.82                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1401:G:H2'   | 27:BA:1402:C:H6    | 1.48                     | 0.79              |
| 27:BA:1550:C:H2'   | 27:BA:1551:C:H6    | 1.45                     | 0.79              |
| 27:BA:536:A:H2'    | 27:BA:537:C:C6     | 2.18                     | 0.79              |
| 30:BD:76:PRO:O     | 30:BD:98:VAL:HG23  | 1.83                     | 0.79              |
| 35:BI:12:LEU:HD12  | 35:BI:19:VAL:HG11  | 1.64                     | 0.79              |
| 38:BP:97:PRO:O     | 38:BP:99:LEU:N     | 2.13                     | 0.79              |
| 40:BR:28:LEU:HD12  | 40:BR:48:VAL:HG11  | 1.62                     | 0.79              |
| 42:BT:18:ASP:C     | 42:BT:19:LEU:HD12  | 2.02                     | 0.79              |
| 1:CA:652:U:H1'     | 1:CA:653:A:H2      | 1.48                     | 0.79              |
| 5:CE:42:GLY:HA3    | 5:CE:65:ASN:O      | 1.83                     | 0.79              |
| 27:DA:2123:G:H2'   | 27:DA:2124:G:C8    | 2.17                     | 0.79              |
| 27:DA:246:C:O2'    | 27:DA:247:G:H5'    | 1.83                     | 0.79              |
| 27:DA:956:G:H22    | 27:DA:959:A:H3'    | 1.46                     | 0.79              |
| 44:DV:95:LEU:HD13  | 44:DV:97:LYS:HZ1   | 1.47                     | 0.79              |
| 1:AA:346:G:N3      | 1:AA:346:G:H2'     | 1.98                     | 0.79              |
| 1:AA:735:C:O2'     | 1:AA:736:C:H5'     | 1.81                     | 0.79              |
| 5:AE:50:GLU:HG3    | 5:AE:52:PRO:CD     | 2.05                     | 0.79              |
| 27:BA:1029:A:H2'   | 27:BA:1030:G:H5'   | 1.65                     | 0.79              |
| 27:BA:2777:G:H5''  | 27:BA:2778:A:H5''  | 1.63                     | 0.79              |
| 27:BA:753:C:H2'    | 27:BA:754:C:H5'    | 1.63                     | 0.79              |
| 31:BE:33:VAL:O     | 31:BE:69:LYS:HD2   | 1.82                     | 0.79              |
| 38:BP:71:VAL:CG1   | 38:BP:72:PRO:HD3   | 2.12                     | 0.79              |
| 1:CA:1173:G:H2'    | 1:CA:1174:G:C8     | 2.18                     | 0.79              |
| 27:DA:311:A:H1'    | 27:DA:332:A:C8     | 2.16                     | 0.79              |
| 32:DF:102:PRO:HB2  | 32:DF:105:VAL:HG23 | 1.65                     | 0.79              |
| 28:DB:42:C:O2      | 33:DG:92:VAL:HA    | 1.81                     | 0.79              |
| 1:AA:1245:A:H2'    | 1:AA:1246:C:H6     | 1.46                     | 0.79              |
| 1:AA:141:A:H1'     | 1:AA:182:U:O2      | 1.82                     | 0.79              |
| 1:AA:857:C:H2'     | 1:AA:858:G:O4'     | 1.83                     | 0.79              |
| 8:AH:118:VAL:O     | 8:AH:119:LEU:HD23  | 1.82                     | 0.79              |
| 13:AM:104:ARG:HG2  | 13:AM:105:THR:HG23 | 1.63                     | 0.79              |
| 27:BA:1771:C:O2'   | 27:BA:1786:A:H8    | 1.66                     | 0.79              |
| 27:BA:271(B):C:O2' | 27:BA:271(C):C:H5' | 1.82                     | 0.79              |
| 38:BP:115:LEU:HA   | 38:BP:134:ALA:HB2  | 1.65                     | 0.79              |
| 38:BP:47:ASP:HB3   | 38:BP:48:PRO:CA    | 2.11                     | 0.79              |
| 42:BT:13:ARG:HA    | 42:BT:13:ARG:NH1   | 1.98                     | 0.79              |
| 4:CD:67:ILE:HD13   | 4:CD:196:LEU:HD23  | 1.63                     | 0.79              |
| 13:CM:14:ARG:CZ    | 13:CM:42:ALA:HA    | 2.13                     | 0.79              |
| 27:DA:1187:G:H8    | 27:DA:1187:G:O5'   | 1.65                     | 0.79              |
| 27:DA:2681:C:H5    | 27:DA:2725:A:H62   | 1.28                     | 0.79              |
| 27:DA:345:A:H4'    | 27:DA:346:A:OP1    | 1.82                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:686:G:N2     | 27:DA:788:A:H61    | 1.79                     | 0.79              |
| 27:DA:690:G:H2'    | 27:DA:691:C:H6     | 1.47                     | 0.79              |
| 46:DX:26:TYR:HD2   | 46:DX:92:LEU:HD12  | 1.48                     | 0.79              |
| 7:AG:60:LYS:NZ     | 7:AG:60:LYS:HA     | 1.96                     | 0.79              |
| 27:BA:2432:A:H2'   | 27:BA:2433:A:C8    | 2.18                     | 0.79              |
| 34:BH:85:LYS:NZ    | 34:BH:133:VAL:HG21 | 1.97                     | 0.79              |
| 39:BQ:135:ASP:C    | 39:BQ:137:TYR:H    | 1.84                     | 0.79              |
| 1:CA:1321:C:C5'    | 1:CA:1322:C:H5''   | 2.12                     | 0.79              |
| 53:D4:53:THR:O     | 53:D4:54:LYS:HG2   | 1.82                     | 0.79              |
| 27:DA:1497:U:H5'   | 27:DA:1498:C:H5    | 1.48                     | 0.79              |
| 27:DA:1655:A:H4'   | 31:DE:114:ALA:HA   | 1.63                     | 0.79              |
| 27:DA:2555:U:C2'   | 27:DA:2556:C:H5'   | 2.11                     | 0.79              |
| 27:DA:574:C:H1'    | 27:DA:2055:C:H6    | 1.46                     | 0.79              |
| 31:DE:46:ALA:HA    | 31:DE:82:ARG:O     | 1.81                     | 0.79              |
| 4:AD:9:CYS:H       | 4:AD:22:LYS:NZ     | 1.80                     | 0.79              |
| 27:BA:2103:C:H3'   | 27:BA:2104:G:H5''  | 1.62                     | 0.79              |
| 27:BA:335:C:O2'    | 27:BA:336:C:H5'    | 1.83                     | 0.79              |
| 27:BA:742:G:O2'    | 27:BA:743:G:H5'    | 1.83                     | 0.79              |
| 30:BD:25:THR:HG22  | 30:BD:26:LYS:H     | 1.47                     | 0.79              |
| 38:BP:24:GLY:O     | 38:BP:25:SER:HB3   | 1.83                     | 0.79              |
| 1:CA:1187:G:H4'    | 9:CI:111:ARG:NH1   | 1.98                     | 0.79              |
| 1:CA:155:C:H2'     | 1:CA:156:G:C8      | 2.18                     | 0.79              |
| 1:CA:678:U:H2'     | 1:CA:679:C:C6      | 2.18                     | 0.79              |
| 18:CR:86:VAL:O     | 18:CR:87:ARG:HD3   | 1.82                     | 0.79              |
| 23:CW:35:G:O2'     | 23:CW:36:A:H8      | 1.66                     | 0.79              |
| 27:DA:2290:G:H8    | 27:DA:2290:G:H5'   | 1.46                     | 0.79              |
| 41:DS:97:ARG:HH22  | 41:DS:99:LYS:H     | 1.28                     | 0.79              |
| 1:AA:1137:C:H4'    | 1:AA:1138:G:N2     | 1.98                     | 0.79              |
| 1:AA:153:C:H2'     | 1:AA:154:C:H6      | 1.48                     | 0.79              |
| 3:AC:92:ALA:HB2    | 3:AC:99:VAL:HG11   | 1.65                     | 0.79              |
| 27:BA:1019:U:O2'   | 27:BA:1021:A:H2    | 1.64                     | 0.79              |
| 28:BB:11:C:OP1     | 49:B0:72:ARG:HD2   | 1.82                     | 0.79              |
| 47:BY:96:ILE:HB    | 47:BY:99:CYS:CB    | 2.09                     | 0.79              |
| 1:CA:686:U:O2      | 1:CA:686:U:H2'     | 1.83                     | 0.79              |
| 11:CK:32:ILE:HD11  | 11:CK:41:THR:CG2   | 2.10                     | 0.79              |
| 23:CW:73:C:H2'     | 23:CW:74:C:C5'     | 2.12                     | 0.79              |
| 55:D6:37:ARG:O     | 55:D6:48:VAL:O     | 2.01                     | 0.79              |
| 27:DA:287:C:H6     | 27:DA:287:C:H5'    | 1.48                     | 0.79              |
| 27:DA:948:G:H1     | 27:DA:969:U:H3     | 1.30                     | 0.79              |
| 32:DF:132:VAL:HG22 | 32:DF:133:ASN:OD1  | 1.82                     | 0.79              |
| 41:DS:30:ARG:NH2   | 41:DS:62:LYS:HD2   | 1.98                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:25:ARG:NH1    | 4:AD:30:LYS:HG3    | 1.95                     | 0.79              |
| 6:AF:16:GLN:NE2    | 6:AF:16:GLN:H      | 1.81                     | 0.79              |
| 6:AF:7:ASN:O       | 6:AF:88:VAL:HA     | 1.82                     | 0.79              |
| 27:BA:1482:G:H22   | 27:BA:1507:A:H1'   | 1.46                     | 0.79              |
| 35:BI:114:LEU:HA   | 35:BI:130:TYR:CD1  | 2.18                     | 0.79              |
| 38:BP:16:ARG:HD3   | 38:BP:18:ARG:H     | 1.46                     | 0.79              |
| 27:BA:751:A:O4'    | 45:BW:90:ARG:HG2   | 1.82                     | 0.79              |
| 48:BZ:140:VAL:HG23 | 48:BZ:143:LEU:HD23 | 1.64                     | 0.79              |
| 2:CB:11:LEU:HD12   | 2:CB:217:ARG:NH2   | 1.98                     | 0.79              |
| 27:DA:1767:C:O2'   | 27:DA:1768:U:H5'   | 1.82                     | 0.79              |
| 27:DA:2756:U:H3    | 27:DA:2758:A:H62   | 1.29                     | 0.79              |
| 27:DA:307:G:N2     | 27:DA:309:G:H3'    | 1.98                     | 0.79              |
| 27:DA:744:G:O2'    | 27:DA:745:G:H5'    | 1.83                     | 0.79              |
| 3:AC:50:ALA:HB1    | 3:AC:72:LYS:HB3    | 1.63                     | 0.78              |
| 50:B1:19:GLN:NE2   | 50:B1:19:GLN:HA    | 1.97                     | 0.78              |
| 27:BA:1819:A:H2'   | 30:BD:178:PRO:HB2  | 1.65                     | 0.78              |
| 42:BT:106:SER:HB3  | 42:BT:110:ILE:CD1  | 2.13                     | 0.78              |
| 4:CD:42:GLN:HG2    | 4:CD:42:GLN:O      | 1.80                     | 0.78              |
| 6:CF:75:LEU:O      | 6:CF:79:LEU:HG     | 1.83                     | 0.78              |
| 12:CL:66:TYR:HD2   | 12:CL:67:ILE:N     | 1.81                     | 0.78              |
| 27:DA:1921:G:O2'   | 27:DA:1922:G:H5'   | 1.82                     | 0.78              |
| 30:DD:231:HIS:ND1  | 30:DD:232:PRO:CD   | 2.44                     | 0.78              |
| 34:DH:103:LEU:HD22 | 34:DH:123:PHE:HD2  | 1.48                     | 0.78              |
| 12:AL:76:GLU:O     | 12:AL:77:HIS:HB2   | 1.82                     | 0.78              |
| 20:AT:75:ASN:ND2   | 20:AT:75:ASN:H     | 1.80                     | 0.78              |
| 25:AY:71:A:H2'     | 25:AY:72:G:C8      | 2.18                     | 0.78              |
| 27:BA:2016:U:H2'   | 27:BA:2017:U:C6    | 2.18                     | 0.78              |
| 27:BA:2048:G:H5'   | 27:BA:2048:G:H8    | 1.48                     | 0.78              |
| 27:BA:2870:C:C2'   | 27:BA:2871:C:H5'   | 2.12                     | 0.78              |
| 30:BD:155:LEU:HD23 | 30:BD:177:LEU:HD22 | 1.63                     | 0.78              |
| 38:BP:84:ASN:ND2   | 38:BP:115:LEU:HG   | 1.97                     | 0.78              |
| 39:BQ:1:MET:SD     | 39:BQ:2:LEU:HB2    | 2.24                     | 0.78              |
| 43:BU:27:LEU:HB2   | 43:BU:31:SER:HB3   | 1.64                     | 0.78              |
| 4:CD:33:MET:HA     | 4:CD:33:MET:CE     | 2.13                     | 0.78              |
| 5:CE:76:ILE:HG12   | 5:CE:77:PRO:HD2    | 1.65                     | 0.78              |
| 11:CK:74:ALA:C     | 11:CK:76:GLY:H     | 1.86                     | 0.78              |
| 31:DE:26:ILE:HB    | 31:DE:182:LEU:HB3  | 1.65                     | 0.78              |
| 33:DG:28:VAL:O     | 33:DG:31:VAL:HG12  | 1.82                     | 0.78              |
| 45:DW:72:LYS:HB3   | 45:DW:106:ILE:O    | 1.84                     | 0.78              |
| 47:DY:39:VAL:HG12  | 47:DY:40:GLU:H     | 1.46                     | 0.78              |
| 7:AG:31:MET:HG2    | 7:AG:34:GLY:HA2    | 1.64                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:AO:37:ASN:HD22  | 15:AO:37:ASN:H     | 1.27                     | 0.78              |
| 19:AS:42:PRO:O     | 19:AS:44:MET:SD    | 2.42                     | 0.78              |
| 50:B1:52:ARG:HG3   | 50:B1:53:VAL:H     | 1.48                     | 0.78              |
| 58:B9:29:ASN:H     | 58:B9:29:ASN:ND2   | 1.77                     | 0.78              |
| 27:BA:30:G:H2'     | 27:BA:31:C:C6      | 2.19                     | 0.78              |
| 28:BB:4:C:H42      | 28:BB:117:G:H1     | 1.27                     | 0.78              |
| 31:BE:50:GLY:HA2   | 31:BE:78:LEU:HB3   | 1.65                     | 0.78              |
| 32:BF:32:LEU:HD21  | 32:BF:105:VAL:HG13 | 1.63                     | 0.78              |
| 27:BA:71:A:H2      | 46:BX:31:HIS:CE1   | 2.01                     | 0.78              |
| 48:BZ:13:LYS:HB3   | 48:BZ:16:ALA:HB3   | 1.65                     | 0.78              |
| 1:CA:1251:A:H2'    | 1:CA:1252:A:C8     | 2.18                     | 0.78              |
| 1:CA:1343:G:H4'    | 9:CI:122:ALA:HB3   | 1.64                     | 0.78              |
| 1:CA:471:G:HO2'    | 1:CA:472:A:H8      | 0.79                     | 0.78              |
| 12:CL:66:TYR:HD1   | 12:CL:87:VAL:HG21  | 1.48                     | 0.78              |
| 13:CM:95:GLY:O     | 13:CM:96:LEU:HB2   | 1.81                     | 0.78              |
| 27:DA:154(A):C:H41 | 27:DA:172:C:N4     | 1.79                     | 0.78              |
| 27:DA:1984:G:O2'   | 27:DA:1985:G:H5'   | 1.84                     | 0.78              |
| 27:DA:2070:G:H2'   | 27:DA:2071:A:C8    | 2.17                     | 0.78              |
| 27:DA:2061:G:OP2   | 27:DA:2502:G:H5'   | 1.83                     | 0.78              |
| 27:DA:1782:C:H42   | 27:DA:2586:C:H42   | 1.31                     | 0.78              |
| 32:DF:78:ILE:HA    | 32:DF:83:PHE:CD1   | 2.18                     | 0.78              |
| 50:B1:86:SER:HB2   | 50:B1:89:GLU:HB2   | 1.65                     | 0.78              |
| 58:B9:14:CYS:O     | 58:B9:15:LYS:HB2   | 1.81                     | 0.78              |
| 27:BA:271(S):G:H2' | 27:BA:271(T):C:H5' | 1.64                     | 0.78              |
| 31:BE:116:VAL:O    | 31:BE:117:MET:HB3  | 1.82                     | 0.78              |
| 38:BP:144:GLU:H    | 38:BP:145:PRO:HD3  | 1.48                     | 0.78              |
| 17:CQ:81:ARG:HH11  | 17:CQ:84:LEU:HD11  | 1.48                     | 0.78              |
| 24:CX:10:G:N2      | 24:CX:26:G:H1'     | 1.98                     | 0.78              |
| 27:DA:2197:U:O2'   | 27:DA:2198:A:H2'   | 1.82                     | 0.78              |
| 27:DA:704:G:C2'    | 27:DA:726:G:H22    | 1.93                     | 0.78              |
| 27:DA:980:A:O2'    | 27:DA:981:A:H5'    | 1.82                     | 0.78              |
| 28:DB:16:G:H1      | 28:DB:68:C:H42     | 1.31                     | 0.78              |
| 48:DZ:27:MET:HE3   | 48:DZ:34:ARG:HB2   | 1.66                     | 0.78              |
| 1:AA:1136:U:H5''   | 1:AA:1137:C:C5     | 2.19                     | 0.78              |
| 1:AA:643:C:O2'     | 1:AA:644:G:H5'     | 1.84                     | 0.78              |
| 12:AL:72:HIS:HB3   | 12:AL:99:ARG:HH12  | 1.49                     | 0.78              |
| 27:BA:1411:C:H2'   | 27:BA:1412:A:C8    | 2.19                     | 0.78              |
| 27:BA:2065:C:H2'   | 27:BA:2066:C:H6    | 1.47                     | 0.78              |
| 29:BC:196:LEU:C    | 29:BC:198:ALA:H    | 1.87                     | 0.78              |
| 1:CA:1132:C:O2'    | 1:CA:1133:G:H5'    | 1.84                     | 0.78              |
| 10:CJ:9:ARG:HH21   | 10:CJ:95:GLU:HG2   | 1.49                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DX:60:ARG:NH2   | 56:D7:47:ARG:CZ    | 2.47                     | 0.78              |
| 57:D8:21:LYS:HD3   | 57:D8:48:PHE:CZ    | 2.18                     | 0.78              |
| 38:DP:146:VAL:HG22 | 38:DP:147:LEU:H    | 1.47                     | 0.78              |
| 38:DP:146:VAL:O    | 38:DP:148:LEU:HG   | 1.83                     | 0.78              |
| 42:DT:28:VAL:CG2   | 42:DT:46:GLU:HG3   | 2.13                     | 0.78              |
| 48:DZ:52:ILE:HD12  | 48:DZ:52:ILE:H     | 1.47                     | 0.78              |
| 3:AC:87:LEU:C      | 3:AC:89:GLU:H      | 1.84                     | 0.78              |
| 4:AD:25:ARG:HH12   | 4:AD:30:LYS:CG     | 1.95                     | 0.78              |
| 8:AH:69:ARG:NH1    | 8:AH:76:PRO:HA     | 1.99                     | 0.78              |
| 10:AJ:63:PHE:HA    | 14:AN:59:ALA:HB3   | 1.66                     | 0.78              |
| 27:BA:2702:U:H4'   | 27:BA:2703:C:OP1   | 1.83                     | 0.78              |
| 32:BF:132:VAL:HG13 | 32:BF:133:ASN:N    | 1.97                     | 0.78              |
| 42:BT:65:LYS:HE3   | 42:BT:66:VAL:H     | 1.45                     | 0.78              |
| 44:BV:13:ARG:HH11  | 44:BV:13:ARG:HG2   | 1.49                     | 0.78              |
| 44:BV:38:LEU:C     | 44:BV:38:LEU:HD23  | 2.04                     | 0.78              |
| 1:CA:1338:G:H2'    | 1:CA:1339:A:C8     | 2.19                     | 0.78              |
| 27:DA:2034:U:O2'   | 27:DA:2035:G:H5'   | 1.83                     | 0.78              |
| 27:DA:2473:U:O2    | 27:DA:2473:U:H2'   | 1.81                     | 0.78              |
| 27:DA:2481:G:H4'   | 27:DA:2482:G:H5'   | 1.66                     | 0.78              |
| 27:DA:581:C:H2'    | 27:DA:582:G:C8     | 2.18                     | 0.78              |
| 31:DE:179:GLU:HB3  | 31:DE:181:LEU:CD1  | 2.13                     | 0.78              |
| 31:DE:2:LYS:HE2    | 31:DE:95:ILE:CG2   | 2.14                     | 0.78              |
| 2:AB:69:LEU:HD23   | 2:AB:159:PRO:HG2   | 1.66                     | 0.78              |
| 1:AA:472:A:H4'     | 16:AP:80:PHE:O     | 1.83                     | 0.78              |
| 27:BA:258:G:O2'    | 27:BA:259:G:H5'    | 1.83                     | 0.78              |
| 32:BF:165:ARG:HA   | 32:BF:168:ARG:HD2  | 1.66                     | 0.78              |
| 39:BQ:118:LEU:HD13 | 39:BQ:131:ILE:HG23 | 1.64                     | 0.78              |
| 2:CB:44:LEU:H      | 2:CB:44:LEU:HD12   | 1.48                     | 0.78              |
| 1:CA:1321:C:H4'    | 13:CM:87:TYR:CE2   | 2.18                     | 0.78              |
| 27:DA:2527:C:H5'   | 58:D9:30:PRO:HB2   | 1.65                     | 0.78              |
| 27:DA:2543:G:H2'   | 27:DA:2544:G:C8    | 2.19                     | 0.78              |
| 27:DA:2554:U:C6    | 27:DA:2555:U:H5    | 2.02                     | 0.78              |
| 37:DO:35:VAL:HG22  | 37:DO:65:THR:HG21  | 1.65                     | 0.78              |
| 27:DA:627:A:H62    | 38:DP:84:ASN:HD21  | 1.31                     | 0.78              |
| 31:DE:111:ARG:HA   | 40:DR:2:ARG:HG3    | 1.63                     | 0.78              |
| 42:DT:35:LYS:HZ3   | 42:DT:41:ARG:HE    | 1.31                     | 0.78              |
| 1:AA:601:C:O2'     | 1:AA:602:A:H5'     | 1.84                     | 0.78              |
| 4:AD:155:LEU:O     | 4:AD:159:ARG:HG2   | 1.84                     | 0.78              |
| 2:AB:181:PHE:CE1   | 8:AH:70:GLN:HB2    | 2.19                     | 0.78              |
| 18:AR:53:ARG:HH21  | 18:AR:60:ALA:H     | 1.31                     | 0.78              |
| 55:B6:10:LEU:HD12  | 57:B8:34:TRP:HD1   | 1.49                     | 0.78              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:1020:A:N1    | 27:BA:1141:U:O2'  | 2.16                     | 0.78              |
| 27:BA:1490:A:H2'   | 27:BA:1490:A:N3   | 1.99                     | 0.78              |
| 27:BA:344:G:N2     | 27:BA:345:A:H62   | 1.81                     | 0.78              |
| 27:BA:484:C:H2'    | 27:BA:485:C:C6    | 2.19                     | 0.78              |
| 31:BE:184:VAL:HG12 | 31:BE:185:LYS:N   | 1.98                     | 0.78              |
| 31:BE:203:LYS:O    | 31:BE:203:LYS:HD2 | 1.84                     | 0.78              |
| 36:BN:87:LEU:HD21  | 36:BN:98:VAL:HG11 | 1.65                     | 0.78              |
| 47:BY:38:ILE:HG22  | 47:BY:39:VAL:N    | 1.97                     | 0.78              |
| 1:CA:1002:G:N2     | 1:CA:1003:G:H1'   | 1.99                     | 0.78              |
| 1:CA:1360:A:H2'    | 1:CA:1361:G:O4'   | 1.84                     | 0.78              |
| 1:CA:562:C:H4'     | 1:CA:563:A:C5'    | 2.13                     | 0.78              |
| 1:CA:652:U:H1'     | 1:CA:653:A:C2     | 2.17                     | 0.78              |
| 16:CP:4:ILE:HG12   | 16:CP:21:VAL:HG23 | 1.65                     | 0.78              |
| 57:D8:4:MET:SD     | 57:D8:61:LEU:HD21 | 2.24                     | 0.78              |
| 27:DA:2483:C:H5'   | 27:DA:2484:G:OP2  | 1.82                     | 0.78              |
| 27:DA:2593:U:H2'   | 27:DA:2594:C:C6   | 2.19                     | 0.78              |
| 27:DA:459:U:H2'    | 27:DA:460:A:H8    | 1.49                     | 0.78              |
| 33:DG:60:LEU:HD12  | 33:DG:68:PRO:HG3  | 1.65                     | 0.78              |
| 36:DN:128:HIS:O    | 36:DN:130:HIS:N   | 2.15                     | 0.78              |
| 46:DX:12:VAL:HG23  | 46:DX:13:LEU:N    | 1.97                     | 0.78              |
| 1:AA:166:G:H2'     | 1:AA:167:G:H8     | 1.45                     | 0.78              |
| 3:AC:150:LYS:HG3   | 3:AC:169:ALA:HB2  | 1.65                     | 0.78              |
| 9:AI:113:LYS:HD3   | 9:AI:119:ALA:O    | 1.83                     | 0.78              |
| 20:AT:26:ASN:HD22  | 20:AT:26:ASN:N    | 1.75                     | 0.78              |
| 42:BT:26:ASP:HB3   | 42:BT:89:VAL:O    | 1.84                     | 0.78              |
| 42:BT:89:VAL:CG1   | 42:BT:91:ARG:HG2  | 2.13                     | 0.78              |
| 1:CA:689:C:H2'     | 1:CA:690:G:O4'    | 1.82                     | 0.78              |
| 1:CA:896:C:O2'     | 1:CA:897:C:H5'    | 1.83                     | 0.78              |
| 7:CG:46:ALA:O      | 7:CG:50:ILE:HG12  | 1.83                     | 0.78              |
| 55:D6:11:LEU:HD13  | 55:D6:12:GLU:H    | 1.49                     | 0.78              |
| 38:DP:47:ASP:HB3   | 38:DP:48:PRO:CA   | 2.12                     | 0.78              |
| 39:DQ:39:PRO:HD3   | 39:DQ:99:PRO:HG3  | 1.64                     | 0.78              |
| 9:AI:99:LEU:HB3    | 9:AI:101:PHE:CE1  | 2.18                     | 0.78              |
| 11:AK:125:PHE:H    | 11:AK:125:PHE:HD1 | 1.30                     | 0.78              |
| 11:AK:28:THR:HG21  | 11:AK:61:ALA:HB1  | 1.66                     | 0.78              |
| 14:AN:29:ARG:HH12  | 14:AN:31:ARG:HB2  | 1.47                     | 0.78              |
| 27:BA:1401:G:H2'   | 27:BA:1402:C:C6   | 2.18                     | 0.78              |
| 27:BA:2439:A:H5'   | 27:BA:2439:A:H8   | 1.48                     | 0.78              |
| 27:BA:740:U:H5'    | 27:BA:740:U:C6    | 2.17                     | 0.78              |
| 27:BA:779:U:OP1    | 30:BD:49:ILE:HG22 | 1.83                     | 0.78              |
| 44:BV:18:LEU:HD13  | 44:BV:19:LYS:N    | 1.98                     | 0.78              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BX:49:VAL:HG23 | 46:BX:50:LYS:N     | 1.99                     | 0.78              |
| 3:CC:22:TRP:HZ3   | 3:CC:32:LEU:HB3    | 1.48                     | 0.78              |
| 4:CD:198:VAL:HG12 | 4:CD:199:ASN:N     | 1.96                     | 0.78              |
| 19:CS:20:LEU:HA   | 19:CS:23:ASN:HD22  | 1.49                     | 0.78              |
| 27:DA:226:G:HO2'  | 27:DA:227:A:H8     | 1.29                     | 0.78              |
| 27:DA:2848:G:H4'  | 27:DA:2849:U:OP1   | 1.84                     | 0.78              |
| 27:DA:330:A:O2'   | 27:DA:331:A:H8     | 1.67                     | 0.78              |
| 38:DP:34:GLY:O    | 38:DP:35:HIS:HB2   | 1.84                     | 0.78              |
| 8:AH:69:ARG:HH12  | 8:AH:76:PRO:HA     | 1.49                     | 0.77              |
| 10:AJ:96:ILE:HD13 | 10:AJ:96:ILE:N     | 1.99                     | 0.77              |
| 13:AM:50:GLU:O    | 13:AM:54:VAL:HG23  | 1.83                     | 0.77              |
| 13:AM:79:LYS:O    | 13:AM:82:MET:HB3   | 1.84                     | 0.77              |
| 27:BA:587:C:H6    | 27:BA:587:C:O5'    | 1.66                     | 0.77              |
| 30:BD:72:LYS:HD3  | 30:BD:75:ILE:HD12  | 1.65                     | 0.77              |
| 33:BG:36:LYS:HD3  | 33:BG:95:ARG:HH12  | 1.49                     | 0.77              |
| 1:CA:1058:G:H2'   | 1:CA:1059:C:C6     | 2.18                     | 0.77              |
| 1:CA:507:C:H3'    | 1:CA:508:C:C6      | 2.19                     | 0.77              |
| 7:CG:78:ARG:HG3   | 7:CG:79:ARG:N      | 1.98                     | 0.77              |
| 13:CM:13:LYS:CA   | 13:CM:44:ARG:HH11  | 1.96                     | 0.77              |
| 55:D6:19:ARG:HG2  | 55:D6:20:ASN:H     | 1.48                     | 0.77              |
| 27:DA:1512:U:H2'  | 27:DA:1513:C:C6    | 2.19                     | 0.77              |
| 27:DA:2532:G:H22  | 27:DA:2663:G:H1'   | 1.48                     | 0.77              |
| 27:DA:953:A:O2'   | 27:DA:954:G:H5'    | 1.83                     | 0.77              |
| 32:DF:9:ILE:HA    | 32:DF:13:SER:O     | 1.83                     | 0.77              |
| 35:DI:60:GLU:O    | 35:DI:64:GLU:HG2   | 1.84                     | 0.77              |
| 38:DP:144:GLU:N   | 38:DP:145:PRO:CD   | 2.47                     | 0.77              |
| 34:BH:98:LEU:O    | 34:BH:99:VAL:HG23  | 1.84                     | 0.77              |
| 40:BR:104:ARG:O   | 40:BR:108:GLY:HA2  | 1.84                     | 0.77              |
| 3:CC:24:ALA:HB1   | 3:CC:32:LEU:HD12   | 1.66                     | 0.77              |
| 13:CM:25:ILE:CD1  | 13:CM:66:LEU:HD23  | 2.10                     | 0.77              |
| 15:CO:69:TYR:CE2  | 15:CO:73:GLU:HG3   | 2.19                     | 0.77              |
| 27:DA:1481:U:H5'  | 27:DA:1482:G:OP2   | 1.84                     | 0.77              |
| 28:DB:28:C:H2'    | 28:DB:29:A:H8      | 1.48                     | 0.77              |
| 42:DT:57:PHE:CG   | 42:DT:58:ASN:N     | 2.50                     | 0.77              |
| 37:DO:71:ARG:HH12 | 42:DT:74:ARG:HH22  | 1.32                     | 0.77              |
| 48:DZ:149:LEU:CD2 | 48:DZ:170:ILE:HG13 | 2.13                     | 0.77              |
| 48:DZ:54:HIS:NE2  | 48:DZ:134:GLU:HA   | 2.00                     | 0.77              |
| 7:AG:50:ILE:HG22  | 7:AG:56:GLN:O      | 1.84                     | 0.77              |
| 24:AX:2:G:H2'     | 24:AX:3:C:H6       | 1.50                     | 0.77              |
| 44:BV:49:THR:HG22 | 44:BV:50:PRO:HD3   | 1.66                     | 0.77              |
| 1:CA:1187:G:H4'   | 9:CI:111:ARG:HH11  | 1.50                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:982:U:H5''   | 14:CN:6:LEU:HD11   | 1.65                     | 0.77              |
| 27:DA:2037:G:H2'  | 27:DA:2038:G:H8    | 1.50                     | 0.77              |
| 30:DD:30:GLU:HG3  | 30:DD:63:ARG:CZ    | 2.15                     | 0.77              |
| 32:DF:10:PRO:HD2  | 32:DF:13:SER:O     | 1.84                     | 0.77              |
| 1:AA:221:C:O2'    | 1:AA:222:U:H5'     | 1.85                     | 0.77              |
| 7:AG:116:ALA:HA   | 7:AG:119:ARG:HE    | 1.49                     | 0.77              |
| 1:AA:823:G:H21    | 8:AH:1:MET:HE1     | 1.48                     | 0.77              |
| 24:AX:4:G:H2'     | 24:AX:5:G:H8       | 1.45                     | 0.77              |
| 27:BA:1490:A:H5'  | 27:BA:1491:G:OP2   | 1.84                     | 0.77              |
| 27:BA:2836:U:H2'  | 27:BA:2837:G:H8    | 1.43                     | 0.77              |
| 37:BO:8:LEU:CD1   | 37:BO:82:ASN:HB3   | 2.14                     | 0.77              |
| 37:BO:87:ILE:HG22 | 37:BO:88:ASN:O     | 1.84                     | 0.77              |
| 1:CA:763:G:H2'    | 1:CA:764:C:C6      | 2.17                     | 0.77              |
| 2:CB:158:LEU:HD12 | 2:CB:158:LEU:N     | 1.99                     | 0.77              |
| 2:CB:74:LYS:H     | 2:CB:74:LYS:HD2    | 1.50                     | 0.77              |
| 23:CW:2:G:H2'     | 23:CW:3:G:O4'      | 1.85                     | 0.77              |
| 38:DP:50:ARG:HB3  | 57:D8:59:LYS:CD    | 2.14                     | 0.77              |
| 27:DA:2370:G:H21  | 55:D6:45:LYS:HZ1   | 1.28                     | 0.77              |
| 1:AA:939:G:H5''   | 7:AG:102:ARG:NH1   | 2.00                     | 0.77              |
| 7:AG:151:TYR:HA   | 7:AG:153:HIS:CE1   | 2.19                     | 0.77              |
| 27:BA:111:A:H4'   | 51:B2:69:ARG:NH2   | 1.99                     | 0.77              |
| 27:BA:491:G:H2'   | 27:BA:492:A:C8     | 2.20                     | 0.77              |
| 27:BA:2590:A:OP2  | 30:BD:238:GLY:HA2  | 1.84                     | 0.77              |
| 30:BD:35:LYS:H    | 30:BD:36:PRO:CD    | 1.97                     | 0.77              |
| 33:BG:46:ALA:C    | 33:BG:51:ARG:HG3   | 2.04                     | 0.77              |
| 1:CA:29:G:H1      | 1:CA:554:C:H42     | 1.29                     | 0.77              |
| 1:CA:627:G:H2'    | 1:CA:628:G:H8      | 1.48                     | 0.77              |
| 27:DA:67:U:H2'    | 27:DA:68:G:H8      | 1.49                     | 0.77              |
| 31:DE:134:ILE:H   | 31:DE:134:ILE:HD13 | 1.49                     | 0.77              |
| 37:DO:37:ASP:O    | 37:DO:61:VAL:HA    | 1.83                     | 0.77              |
| 40:DR:10:LEU:HD22 | 40:DR:17:ARG:HD2   | 1.65                     | 0.77              |
| 41:DS:89:ARG:HD2  | 41:DS:92:TYR:HA    | 1.66                     | 0.77              |
| 45:DW:50:VAL:HG13 | 45:DW:51:LEU:H     | 1.49                     | 0.77              |
| 46:DX:12:VAL:HG11 | 46:DX:17:ALA:HB1   | 1.67                     | 0.77              |
| 1:AA:16:A:O2'     | 1:AA:17:U:H5'      | 1.85                     | 0.77              |
| 7:AG:26:PHE:HD1   | 7:AG:101:LEU:HD22  | 1.50                     | 0.77              |
| 15:AO:10:LYS:HG3  | 15:AO:11:VAL:N     | 2.00                     | 0.77              |
| 53:B4:46:ASN:HD22 | 53:B4:47:VAL:H     | 1.31                     | 0.77              |
| 53:B4:46:ASN:HD22 | 53:B4:47:VAL:N     | 1.81                     | 0.77              |
| 27:BA:1175:U:O5'  | 27:BA:1176:G:H5'   | 1.83                     | 0.77              |
| 27:BA:2020:A:O2'  | 27:BA:2021:C:H3'   | 1.84                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2123:G:H2'  | 27:BA:2124:G:H8    | 1.50                     | 0.77              |
| 27:BA:626:U:H5'   | 27:BA:627:A:C5'    | 2.15                     | 0.77              |
| 27:BA:693:C:O2'   | 27:BA:694:U:H5'    | 1.85                     | 0.77              |
| 32:BF:61:GLY:O    | 32:BF:77:ASP:HB3   | 1.82                     | 0.77              |
| 33:BG:112:PRO:C   | 33:BG:113:ARG:HH11 | 1.86                     | 0.77              |
| 36:BN:76:SER:O    | 36:BN:78:TYR:N     | 2.17                     | 0.77              |
| 47:BY:2:ARG:HD3   | 47:BY:3:VAL:HG23   | 1.65                     | 0.77              |
| 48:BZ:52:ILE:HG23 | 48:BZ:70:VAL:HB    | 1.62                     | 0.77              |
| 1:CA:222:U:H2'    | 1:CA:223:U:C6      | 2.19                     | 0.77              |
| 5:CE:78:HIS:O     | 5:CE:93:PRO:HD3    | 1.84                     | 0.77              |
| 8:CH:108:GLY:HA3  | 8:CH:138:TRP:HB3   | 1.65                     | 0.77              |
| 1:CA:192:U:H4'    | 20:CT:103:GLY:HA2  | 1.66                     | 0.77              |
| 51:D2:47:ASN:O    | 51:D2:49:LYS:N     | 2.16                     | 0.77              |
| 55:D6:40:CYS:HA   | 55:D6:46:HIS:CB    | 2.13                     | 0.77              |
| 27:DA:1689:A:N6   | 27:DA:1698:A:H2    | 1.79                     | 0.77              |
| 27:DA:2870:C:C2'  | 27:DA:2871:C:H5'   | 2.14                     | 0.77              |
| 27:DA:704:G:C2'   | 27:DA:726:G:N2     | 2.48                     | 0.77              |
| 32:DF:33:LEU:HD11 | 32:DF:109:GLY:HA2  | 1.66                     | 0.77              |
| 39:DQ:27:VAL:HG12 | 39:DQ:29:PHE:H     | 1.50                     | 0.77              |
| 40:DR:76:VAL:O    | 40:DR:79:LEU:HB3   | 1.84                     | 0.77              |
| 44:DV:40:LEU:HD13 | 44:DV:46:VAL:HA    | 1.66                     | 0.77              |
| 1:AA:1076:C:H42   | 1:AA:1081:G:H1     | 1.33                     | 0.77              |
| 1:AA:1158:C:H2'   | 1:AA:1158:C:O2     | 1.82                     | 0.77              |
| 38:BP:63:PRO:HB3  | 57:B8:13:ARG:HB3   | 1.67                     | 0.77              |
| 27:BA:1278:A:O2'  | 27:BA:1279:G:H5'   | 1.85                     | 0.77              |
| 32:BF:67:GLN:O    | 32:BF:68:LYS:HB2   | 1.83                     | 0.77              |
| 37:BO:19:ILE:HG22 | 37:BO:43:VAL:HG13  | 1.65                     | 0.77              |
| 13:CM:82:MET:HG2  | 13:CM:82:MET:O     | 1.83                     | 0.77              |
| 50:D1:80:LEU:HD13 | 50:D1:82:LEU:HD21  | 1.63                     | 0.77              |
| 27:DA:414:C:H2'   | 27:DA:415:A:H8     | 1.47                     | 0.77              |
| 33:DG:111:LEU:CD1 | 33:DG:120:LEU:HD21 | 2.14                     | 0.77              |
| 33:DG:152:LEU:O   | 33:DG:153:ARG:HD3  | 1.83                     | 0.77              |
| 36:DN:86:PRO:HG2  | 36:DN:89:LYS:HG2   | 1.66                     | 0.77              |
| 36:DN:4:TYR:HB2   | 43:DU:64:ARG:NH1   | 1.99                     | 0.77              |
| 27:DA:328:U:H4'   | 47:DY:68:HIS:ND1   | 1.99                     | 0.77              |
| 1:AA:1366:C:H2'   | 1:AA:1367:C:H6     | 1.49                     | 0.77              |
| 5:AE:129:ILE:O    | 5:AE:131:ILE:N     | 2.18                     | 0.77              |
| 8:AH:63:LEU:CB    | 8:AH:65:TYR:HE1    | 1.97                     | 0.77              |
| 10:AJ:6:ILE:HG13  | 10:AJ:72:VAL:O     | 1.84                     | 0.77              |
| 11:AK:20:TYR:C    | 11:AK:21:ILE:HD12  | 2.04                     | 0.77              |
| 52:B3:29:ARG:CB   | 52:B3:33:GLN:HE22  | 1.98                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:BF:10:PRO:HG2   | 32:BF:11:VAL:HG23  | 1.65                     | 0.77              |
| 32:BF:53:THR:HB    | 32:BF:56:GLU:HG3   | 1.67                     | 0.77              |
| 48:BZ:162:LEU:CD2  | 48:BZ:166:PRO:HG3  | 2.15                     | 0.77              |
| 1:CA:1347:G:H22    | 1:CA:1373:G:C2'    | 1.93                     | 0.77              |
| 27:DA:1473:G:H2'   | 27:DA:1474:C:H5'   | 1.66                     | 0.77              |
| 42:DT:16:ARG:O     | 42:DT:17:THR:HB    | 1.85                     | 0.77              |
| 45:DW:68:ARG:HH12  | 45:DW:113:LYS:H    | 1.31                     | 0.77              |
| 45:DW:17:VAL:O     | 45:DW:20:VAL:N     | 2.16                     | 0.77              |
| 46:DX:12:VAL:HG12  | 46:DX:27:THR:OG1   | 1.83                     | 0.77              |
| 1:AA:1510:U:H2'    | 1:AA:1511:G:C8     | 2.20                     | 0.77              |
| 1:AA:308:C:H2'     | 1:AA:309:G:H8      | 1.49                     | 0.77              |
| 15:AO:78:TYR:OH    | 15:AO:88:ARG:HD2   | 1.83                     | 0.77              |
| 53:B4:62:CYS:SG    | 53:B4:64:LYS:HG3   | 2.25                     | 0.77              |
| 55:B6:20:ASN:OD1   | 55:B6:41:PRO:HA    | 1.85                     | 0.77              |
| 27:BA:143:G:H1'    | 46:BX:37:THR:HG21  | 1.65                     | 0.77              |
| 1:CA:1151:A:H1'    | 10:CJ:39:PRO:HG2   | 1.64                     | 0.77              |
| 1:CA:1267:C:H2'    | 1:CA:1267:C:O2     | 1.84                     | 0.77              |
| 1:CA:1332:A:H2'    | 1:CA:1333:A:C8     | 2.20                     | 0.77              |
| 4:CD:201:GLN:HA    | 4:CD:201:GLN:OE1   | 1.84                     | 0.77              |
| 54:D5:32:PRO:O     | 54:D5:33:CYS:HB3   | 1.83                     | 0.77              |
| 27:DA:1153:C:H2'   | 27:DA:1154:G:O4'   | 1.85                     | 0.77              |
| 31:DE:7:VAL:HG23   | 31:DE:27:LEU:HB3   | 1.67                     | 0.77              |
| 32:DF:182:ASN:O    | 32:DF:186:ILE:HG12 | 1.85                     | 0.77              |
| 27:BA:518:G:H2'    | 27:BA:519:U:C6     | 2.20                     | 0.77              |
| 30:BD:43:ARG:HH11  | 30:BD:44:ASN:ND2   | 1.82                     | 0.77              |
| 20:CT:76:ALA:HA    | 20:CT:79:ARG:HH11  | 1.49                     | 0.77              |
| 25:CY:37:U:C3'     | 25:CY:38:U:H5''    | 2.15                     | 0.77              |
| 55:D6:11:LEU:HD11  | 55:D6:52:VAL:O     | 1.83                     | 0.77              |
| 27:DA:2716:U:O2'   | 27:DA:2717:G:H5'   | 1.85                     | 0.77              |
| 27:DA:473:G:H5''   | 27:DA:508:G:N2     | 1.99                     | 0.77              |
| 38:DP:115:LEU:HD23 | 38:DP:115:LEU:N    | 2.00                     | 0.77              |
| 38:DP:23:PRO:HB2   | 38:DP:33:ARG:CD    | 2.14                     | 0.77              |
| 38:DP:91:PHE:N     | 38:DP:91:PHE:CD1   | 2.51                     | 0.77              |
| 43:DU:88:ILE:O     | 43:DU:88:ILE:HG13  | 1.82                     | 0.77              |
| 1:AA:1207:G:H2'    | 1:AA:1208:C:C6     | 2.20                     | 0.76              |
| 4:AD:119:GLN:HE21  | 4:AD:123:HIS:CD2   | 2.03                     | 0.76              |
| 6:AF:55:ASP:HB3    | 6:AF:86:ARG:HH12   | 1.50                     | 0.76              |
| 27:BA:1656:C:O2'   | 27:BA:1657:C:H5'   | 1.84                     | 0.76              |
| 27:BA:90:U:H1'     | 27:BA:92:A:C8      | 2.20                     | 0.76              |
| 41:BS:13:ARG:O     | 41:BS:15:ARG:HG2   | 1.84                     | 0.76              |
| 1:CA:1037:C:H2'    | 1:CA:1038:C:C6     | 2.19                     | 0.76              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:226:G:O2'     | 1:CA:227:G:H5'    | 1.85                     | 0.76              |
| 19:CS:40:ILE:HG21  | 19:CS:62:ILE:HD11 | 1.66                     | 0.76              |
| 27:DA:1284:A:H2'   | 27:DA:1285:G:O4'  | 1.85                     | 0.76              |
| 27:DA:2629:A:N3    | 27:DA:2629:A:H5'  | 1.99                     | 0.76              |
| 27:DA:774:A:H2     | 27:DA:787:U:HO2'  | 1.33                     | 0.76              |
| 33:DG:43:LEU:CB    | 33:DG:88:ILE:HD11 | 2.15                     | 0.76              |
| 44:DV:19:LYS:HB2   | 44:DV:96:ILE:HG12 | 1.67                     | 0.76              |
| 43:DU:89:GLU:CG    | 44:DV:50:PRO:HG3  | 2.14                     | 0.76              |
| 1:AA:1528:U:HO2'   | 1:AA:1529:G:H3'   | 1.50                     | 0.76              |
| 4:AD:170:VAL:HG12  | 4:AD:171:GLY:N    | 2.00                     | 0.76              |
| 1:AA:1377:A:H2'    | 7:AG:7:ALA:HB3    | 1.67                     | 0.76              |
| 27:BA:594:U:H2'    | 27:BA:595:C:H6    | 1.50                     | 0.76              |
| 31:BE:203:LYS:HE3  | 31:BE:204:ALA:HB2 | 1.66                     | 0.76              |
| 32:BF:46:ARG:HB3   | 32:BF:48:THR:HG23 | 1.67                     | 0.76              |
| 37:BO:13:ASN:HD21  | 37:BO:96:THR:C    | 1.87                     | 0.76              |
| 38:BP:146:VAL:HG22 | 38:BP:147:LEU:N   | 2.01                     | 0.76              |
| 42:BT:99:LEU:O     | 42:BT:99:LEU:HD12 | 1.84                     | 0.76              |
| 1:CA:1149:C:H2'    | 1:CA:1150:U:C6    | 2.20                     | 0.76              |
| 9:CI:13:ALA:HB2    | 9:CI:68:GLY:HA3   | 1.68                     | 0.76              |
| 15:CO:54:ARG:NE    | 15:CO:58:MET:SD   | 2.58                     | 0.76              |
| 16:CP:43:LYS:HA    | 16:CP:48:TRP:CB   | 2.15                     | 0.76              |
| 17:CQ:59:ILE:HG22  | 17:CQ:71:PHE:HD1  | 1.50                     | 0.76              |
| 25:CY:63:C:H2'     | 25:CY:64:G:H8     | 1.50                     | 0.76              |
| 25:CY:65:U:H2'     | 25:CY:66:A:C8     | 2.21                     | 0.76              |
| 27:DA:1384:A:N3    | 27:DA:1405:U:H1'  | 2.00                     | 0.76              |
| 29:DC:77:ILE:HB    | 29:DC:122:ALA:HA  | 1.65                     | 0.76              |
| 31:DE:105:THR:HG21 | 31:DE:164:ARG:CZ  | 2.15                     | 0.76              |
| 33:DG:101:ILE:HD11 | 33:DG:105:LYS:HZ1 | 1.50                     | 0.76              |
| 39:DQ:32:TYR:CE2   | 39:DQ:133:ARG:HG2 | 2.19                     | 0.76              |
| 39:DQ:63:LYS:HE2   | 39:DQ:65:PHE:CE1  | 2.19                     | 0.76              |
| 4:AD:4:TYR:O       | 4:AD:5:ILE:HB     | 1.85                     | 0.76              |
| 6:AF:21:LEU:O      | 6:AF:24:GLU:HG2   | 1.86                     | 0.76              |
| 11:AK:12:ARG:HE    | 11:AK:14:VAL:HG12 | 1.49                     | 0.76              |
| 27:BA:2611:U:H5'   | 27:BA:2611:U:H6   | 1.50                     | 0.76              |
| 27:BA:627:A:H4'    | 27:BA:628:G:OP1   | 1.84                     | 0.76              |
| 30:BD:134:ARG:HD3  | 30:BD:135:PHE:CZ  | 2.21                     | 0.76              |
| 32:BF:4:VAL:HG12   | 32:BF:19:GLU:OE1  | 1.86                     | 0.76              |
| 35:BI:133:HIS:HB2  | 35:BI:134:PRO:CD  | 2.15                     | 0.76              |
| 36:BN:2:LYS:NZ     | 43:BU:95:LEU:HG   | 1.99                     | 0.76              |
| 43:BU:92:ARG:HG2   | 44:BV:11:GLN:CD   | 2.06                     | 0.76              |
| 1:CA:1427:U:H2'    | 1:CA:1428:A:C8    | 2.21                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:321:A:O2'    | 1:CA:322:C:H5'    | 1.84                     | 0.76              |
| 1:CA:784:C:H4'    | 27:DA:1837:C:OP1  | 1.85                     | 0.76              |
| 11:CK:101:SER:C   | 11:CK:103:LEU:H   | 1.87                     | 0.76              |
| 12:CL:25:LYS:HE3  | 12:CL:30:ARG:HH12 | 1.50                     | 0.76              |
| 23:CW:14:A:H2'    | 23:CW:15:G:O4'    | 1.85                     | 0.76              |
| 27:DA:2399:G:H21  | 55:D6:21:TYR:HE1  | 1.30                     | 0.76              |
| 27:DA:1213:A:H2'  | 27:DA:1214:A:H8   | 1.48                     | 0.76              |
| 27:DA:1378:A:H4'  | 27:DA:1379:A:OP1  | 1.83                     | 0.76              |
| 27:DA:2571:C:C5'  | 27:DA:2572:A:H5'  | 2.14                     | 0.76              |
| 27:DA:459:U:H4'   | 56:D7:40:TRP:CZ3  | 2.19                     | 0.76              |
| 27:DA:528:A:C2    | 27:DA:2043:C:H4'  | 2.20                     | 0.76              |
| 31:DE:33:VAL:CG2  | 31:DE:69:LYS:HE3  | 2.15                     | 0.76              |
| 37:DO:66:LYS:HD3  | 37:DO:79:PHE:O    | 1.84                     | 0.76              |
| 1:AA:1256:A:H5'   | 1:AA:1257:U:OP1   | 1.84                     | 0.76              |
| 1:AA:577:G:O2'    | 1:AA:578:C:H6     | 1.69                     | 0.76              |
| 3:AC:43:LEU:O     | 3:AC:47:LEU:HB3   | 1.84                     | 0.76              |
| 19:AS:4:SER:O     | 19:AS:5:LEU:HB2   | 1.83                     | 0.76              |
| 27:BA:2863:C:C2'  | 27:BA:2864:G:H5'' | 2.15                     | 0.76              |
| 27:BA:675:A:C8    | 27:BA:804:A:C6    | 2.73                     | 0.76              |
| 1:CA:197:A:N6     | 1:CA:221:C:H5'    | 2.01                     | 0.76              |
| 1:CA:678:U:H2'    | 1:CA:679:C:H6     | 1.49                     | 0.76              |
| 1:CA:924:C:H2'    | 1:CA:925:G:H8     | 1.49                     | 0.76              |
| 1:CA:1057:G:H4'   | 3:CC:196:LEU:O    | 1.85                     | 0.76              |
| 8:CH:39:LEU:HD22  | 8:CH:39:LEU:H     | 1.51                     | 0.76              |
| 8:CH:86:ILE:HG22  | 8:CH:87:SER:H     | 1.51                     | 0.76              |
| 1:CA:1060:C:H5'   | 14:CN:45:ARG:HH22 | 1.50                     | 0.76              |
| 16:CP:82:GLN:NE2  | 16:CP:82:GLN:N    | 2.31                     | 0.76              |
| 27:DA:2532:G:N2   | 27:DA:2663:G:H1'  | 2.00                     | 0.76              |
| 27:DA:2842:G:O2'  | 27:DA:2843:G:H5'  | 1.85                     | 0.76              |
| 27:DA:662:G:H5''  | 38:DP:18:ARG:O    | 1.85                     | 0.76              |
| 36:DN:128:HIS:HB2 | 36:DN:130:HIS:HE1 | 1.46                     | 0.76              |
| 41:DS:92:TYR:O    | 41:DS:93:LYS:HB3  | 1.86                     | 0.76              |
| 1:AA:258:G:H1     | 1:AA:268:C:H42    | 1.33                     | 0.76              |
| 5:AE:141:GLN:HG2  | 5:AE:143:ARG:NH2  | 2.00                     | 0.76              |
| 8:AH:112:LEU:HA   | 8:AH:134:ILE:HG12 | 1.66                     | 0.76              |
| 9:AI:115:GLY:O    | 9:AI:116:LYS:HG2  | 1.85                     | 0.76              |
| 27:BA:2654:A:H4'  | 27:BA:2655:G:OP1  | 1.85                     | 0.76              |
| 1:CA:1175:G:H2'   | 1:CA:1176:A:H8    | 1.50                     | 0.76              |
| 1:CA:1246:C:H2'   | 1:CA:1247:U:H6    | 1.51                     | 0.76              |
| 1:CA:1321:C:H3'   | 1:CA:1322:C:H5''  | 1.67                     | 0.76              |
| 1:CA:269:C:H2'    | 1:CA:270:A:C8     | 2.19                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:310:G:H2'     | 1:CA:311:C:H6      | 1.51                     | 0.76              |
| 27:DA:1484:G:C3'   | 27:DA:1485:G:H5''  | 2.15                     | 0.76              |
| 27:DA:2825:C:H2'   | 27:DA:2826:A:O4'   | 1.85                     | 0.76              |
| 27:DA:363(E):U:H2' | 27:DA:363(E):U:O2  | 1.86                     | 0.76              |
| 27:DA:558:G:OP1    | 36:DN:111:PRO:HD2  | 1.85                     | 0.76              |
| 27:DA:927:G:H2'    | 27:DA:928:G:O4'    | 1.85                     | 0.76              |
| 30:DD:26:LYS:O     | 30:DD:27:THR:HB    | 1.85                     | 0.76              |
| 1:AA:8:A:N7        | 4:AD:208:SER:HB2   | 2.01                     | 0.76              |
| 2:AB:21:ARG:HB3    | 2:AB:39:ILE:HA     | 1.67                     | 0.76              |
| 5:AE:41:VAL:HG11   | 5:AE:113:ALA:HA    | 1.66                     | 0.76              |
| 16:AP:5:ARG:NH2    | 16:AP:26:ARG:HB2   | 1.99                     | 0.76              |
| 27:BA:125:G:H5''   | 27:BA:126:A:OP2    | 1.85                     | 0.76              |
| 27:BA:1372:U:H2'   | 27:BA:1373:A:H8    | 1.49                     | 0.76              |
| 27:BA:1911:U:H2'   | 27:BA:1918:A:N1    | 2.01                     | 0.76              |
| 27:BA:2061:G:H5''  | 27:BA:2503:A:C2    | 2.20                     | 0.76              |
| 31:BE:36:ARG:HH21  | 31:BE:88:GLY:HA3   | 1.48                     | 0.76              |
| 27:BA:1995:U:O2'   | 37:BO:31:LYS:HE3   | 1.86                     | 0.76              |
| 38:BP:122:PRO:HB3  | 38:BP:141:ALA:HB3  | 1.67                     | 0.76              |
| 27:BA:2847:U:OP1   | 42:BT:98:LYS:HD3   | 1.86                     | 0.76              |
| 1:CA:1066:C:H6     | 1:CA:1066:C:H5''   | 1.47                     | 0.76              |
| 1:CA:1332:A:H2'    | 1:CA:1333:A:H8     | 1.51                     | 0.76              |
| 1:CA:1346:A:N1     | 1:CA:1374:A:H5''   | 2.01                     | 0.76              |
| 1:CA:551:U:O2'     | 1:CA:552:U:H5'     | 1.84                     | 0.76              |
| 8:CH:17:THR:HB     | 8:CH:78:GLN:OE1    | 1.85                     | 0.76              |
| 27:DA:1448:G:H2'   | 27:DA:1449:A:C8    | 2.21                     | 0.76              |
| 27:DA:2308:G:H2'   | 27:DA:2309:A:C8    | 2.21                     | 0.76              |
| 27:DA:2712:U:O2'   | 27:DA:2712(A):A:H8 | 1.69                     | 0.76              |
| 29:DC:49:ILE:HD12  | 29:DC:49:ILE:H     | 1.49                     | 0.76              |
| 31:DE:134:ILE:HD13 | 31:DE:134:ILE:N    | 1.99                     | 0.76              |
| 33:DG:76:SER:HA    | 33:DG:83:ARG:HB2   | 1.68                     | 0.76              |
| 44:DV:18:LEU:CD2   | 44:DV:19:LYS:H     | 1.99                     | 0.76              |
| 45:DW:95:ILE:O     | 45:DW:95:ILE:HG13  | 1.84                     | 0.76              |
| 1:AA:358:U:H2'     | 1:AA:359:U:C6      | 2.21                     | 0.76              |
| 7:AG:60:LYS:HZ3    | 7:AG:60:LYS:HA     | 1.51                     | 0.76              |
| 12:AL:82:ILE:HG23  | 12:AL:95:TYR:HB3   | 1.68                     | 0.76              |
| 27:BA:1430:C:H2'   | 27:BA:1431:U:C6    | 2.20                     | 0.76              |
| 27:BA:2037:G:H2'   | 27:BA:2038:G:C8    | 2.21                     | 0.76              |
| 27:BA:2580:U:C5'   | 31:BE:131:ALA:HB2  | 2.16                     | 0.76              |
| 37:BO:65:THR:HA    | 37:BO:82:ASN:ND2   | 1.99                     | 0.76              |
| 41:BS:54:LEU:HD12  | 41:BS:57:LYS:O     | 1.85                     | 0.76              |
| 43:BU:90:VAL:HG22  | 44:BV:39:LEU:HG    | 1.66                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:123:C:OP1    | 1:CA:312:C:H5'    | 1.86                     | 0.76              |
| 4:CD:30:LYS:C     | 4:CD:32:ALA:H     | 1.89                     | 0.76              |
| 10:CJ:32:ALA:CB   | 10:CJ:76:ASN:HB2  | 2.14                     | 0.76              |
| 27:DA:2094:G:P    | 35:DI:22:LYS:HD2  | 2.26                     | 0.76              |
| 27:DA:2225:A:O2'  | 27:DA:2226:C:OP2  | 2.02                     | 0.76              |
| 27:DA:2836:U:H2'  | 27:DA:2837:G:H8   | 1.51                     | 0.76              |
| 27:DA:36:G:O2'    | 27:DA:37:C:H5'    | 1.85                     | 0.76              |
| 41:DS:85:VAL:N    | 41:DS:106:ARG:HB2 | 1.97                     | 0.76              |
| 36:DN:2:LYS:NZ    | 44:DV:13:ARG:H    | 1.83                     | 0.76              |
| 2:AB:68:ILE:CD1   | 2:AB:161:ALA:HB3  | 2.16                     | 0.76              |
| 1:AA:1377:A:H2'   | 7:AG:7:ALA:CB     | 2.16                     | 0.76              |
| 27:BA:2483:C:C3'  | 27:BA:2484:G:H5'' | 2.14                     | 0.76              |
| 27:BA:2654:A:H1'  | 27:BA:2656:U:C6   | 2.20                     | 0.76              |
| 27:BA:747:U:H5    | 54:B5:3:LYS:HB2   | 1.51                     | 0.76              |
| 30:BD:31:LYS:HG3  | 30:BD:33:LEU:HD13 | 1.68                     | 0.76              |
| 32:BF:3:GLU:CA    | 32:BF:24:LEU:HG   | 2.14                     | 0.76              |
| 34:BH:89:ILE:O    | 34:BH:89:ILE:HD12 | 1.84                     | 0.76              |
| 27:BA:2873:A:C2   | 40:BR:6:SER:HB2   | 2.21                     | 0.76              |
| 41:BS:17:ARG:HA   | 41:BS:20:ARG:HG2  | 1.66                     | 0.76              |
| 1:CA:1308:U:O2'   | 1:CA:1309:G:H5'   | 1.85                     | 0.76              |
| 1:CA:472:A:H2'    | 1:CA:473:G:O4'    | 1.86                     | 0.76              |
| 55:D6:15:GLU:OE1  | 55:D6:43:CYS:HB3  | 1.86                     | 0.76              |
| 27:DA:19:C:OP1    | 43:DU:22:LYS:HD2  | 1.85                     | 0.76              |
| 27:DA:2586:C:C2'  | 27:DA:2587:A:H5'  | 2.16                     | 0.76              |
| 27:DA:1638:C:H1'  | 27:DA:2698:U:O2'  | 1.84                     | 0.76              |
| 29:DC:36:LYS:HB2  | 29:DC:36:LYS:HZ3  | 1.49                     | 0.76              |
| 31:DE:47:VAL:HG21 | 31:DE:86:PRO:HD2  | 1.68                     | 0.76              |
| 43:DU:110:VAL:O   | 43:DU:113:ALA:HB3 | 1.85                     | 0.76              |
| 3:AC:187:ALA:O    | 3:AC:198:VAL:HG23 | 1.84                     | 0.76              |
| 15:AO:17:ARG:HH11 | 15:AO:17:ARG:HG3  | 1.51                     | 0.76              |
| 54:B5:16:ARG:CG   | 54:B5:17:ASP:N    | 2.48                     | 0.76              |
| 54:B5:41:PRO:CG   | 54:B5:44:THR:HG21 | 2.14                     | 0.76              |
| 55:B6:32:ASN:ND2  | 55:B6:33:LYS:H    | 1.84                     | 0.76              |
| 27:BA:1365:A:H5'' | 50:B1:41:ARG:NH2  | 2.01                     | 0.76              |
| 27:BA:1499:C:H2'  | 27:BA:1500:G:H5'  | 1.68                     | 0.76              |
| 27:BA:481:G:H1'   | 27:BA:506:G:N2    | 2.00                     | 0.76              |
| 28:BB:75:G:H5''   | 48:BZ:35:LYS:HE2  | 1.68                     | 0.76              |
| 30:BD:43:ARG:HH12 | 30:BD:44:ASN:HD21 | 1.33                     | 0.76              |
| 32:BF:38:ARG:HH11 | 32:BF:38:ARG:HG3  | 1.50                     | 0.76              |
| 1:CA:1207:G:O2'   | 1:CA:1208:C:H5'   | 1.85                     | 0.76              |
| 1:CA:348:G:H2'    | 1:CA:349:A:H8     | 1.49                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:674:G:H2'     | 1:CA:675:A:H8      | 1.48                     | 0.76              |
| 10:CJ:97:GLU:O     | 10:CJ:98:ILE:HD12  | 1.85                     | 0.76              |
| 14:CN:41:ARG:HG3   | 14:CN:42:ILE:HG12  | 1.67                     | 0.76              |
| 27:DA:1448:G:H2'   | 27:DA:1449:A:H8    | 1.49                     | 0.76              |
| 31:DE:116:VAL:O    | 31:DE:117:MET:HB3  | 1.83                     | 0.76              |
| 31:DE:59:VAL:HG22  | 31:DE:60:ASN:N     | 2.01                     | 0.76              |
| 33:DG:51:ARG:NE    | 33:DG:51:ARG:HA    | 2.00                     | 0.76              |
| 7:AG:80:VAL:HG21   | 7:AG:85:TYR:CD1    | 2.21                     | 0.76              |
| 7:AG:95:ARG:O      | 7:AG:99:LEU:HG     | 1.85                     | 0.76              |
| 8:AH:83:ILE:HG13   | 8:AH:137:VAL:HG22  | 1.68                     | 0.76              |
| 27:BA:1641:A:H2'   | 27:BA:1642:G:O4'   | 1.86                     | 0.76              |
| 27:BA:1913:A:H4'   | 27:BA:1914:C:H5''  | 1.67                     | 0.76              |
| 27:BA:1798:U:C5'   | 30:BD:259:THR:HG22 | 2.14                     | 0.76              |
| 30:BD:35:LYS:NZ    | 30:BD:103:ARG:HA   | 2.01                     | 0.76              |
| 31:BE:46:ALA:HB2   | 31:BE:82:ARG:HA    | 1.68                     | 0.76              |
| 31:BE:1:MET:HB2    | 31:BE:84:PHE:HB2   | 1.68                     | 0.76              |
| 36:BN:57:ALA:O     | 36:BN:58:ASP:O     | 2.04                     | 0.76              |
| 1:CA:1064:G:H1'    | 1:CA:1066:C:C5     | 2.21                     | 0.76              |
| 1:CA:159:G:H2'     | 1:CA:161:A:OP2     | 1.86                     | 0.76              |
| 1:CA:193:C:O2'     | 1:CA:194:C:H5'     | 1.85                     | 0.76              |
| 1:CA:980:C:H5'     | 1:CA:981:U:C5      | 2.21                     | 0.76              |
| 2:CB:107:THR:HA    | 2:CB:110:GLN:HG2   | 1.65                     | 0.76              |
| 3:CC:134:ILE:CG2   | 3:CC:168:ALA:HB3   | 2.15                     | 0.76              |
| 7:CG:85:TYR:HD1    | 7:CG:154:TYR:HE1   | 1.33                     | 0.76              |
| 10:CJ:82:ILE:HG22  | 10:CJ:82:ILE:O     | 1.86                     | 0.76              |
| 27:DA:2113:U:O2'   | 27:DA:2114:A:H8    | 1.69                     | 0.76              |
| 27:DA:586:A:C5'    | 32:DF:89:VAL:HG21  | 2.15                     | 0.76              |
| 31:DE:77:ILE:CG2   | 31:DE:78:LEU:N     | 2.44                     | 0.76              |
| 5:AE:91:LEU:HD12   | 5:AE:120:THR:HG22  | 1.67                     | 0.75              |
| 57:B8:33:ASN:N     | 57:B8:33:ASN:HD22  | 1.82                     | 0.75              |
| 32:BF:3:GLU:HB2    | 32:BF:19:GLU:CB    | 2.09                     | 0.75              |
| 36:BN:62:VAL:HG11  | 36:BN:67:LEU:HD21  | 1.68                     | 0.75              |
| 40:BR:97:VAL:HA    | 40:BR:113:LEU:O    | 1.85                     | 0.75              |
| 43:BU:112:ARG:HH21 | 44:BV:46:VAL:HG11  | 1.50                     | 0.75              |
| 1:CA:507:C:H3'     | 1:CA:508:C:H6      | 1.50                     | 0.75              |
| 3:CC:150:LYS:HD3   | 3:CC:201:TYR:HD1   | 1.51                     | 0.75              |
| 3:CC:22:TRP:CZ3    | 3:CC:32:LEU:HB3    | 2.21                     | 0.75              |
| 7:CG:16:LEU:HD11   | 9:CI:42:ARG:HA     | 1.68                     | 0.75              |
| 16:CP:31:LYS:HG2   | 16:CP:32:TYR:H     | 1.49                     | 0.75              |
| 45:DW:26:GLY:H     | 45:DW:71:VAL:HB    | 1.51                     | 0.75              |
| 1:AA:751:U:C4'     | 15:AO:24:SER:HA    | 2.16                     | 0.75              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:837:G:O2'     | 1:AA:838:G:H5'    | 1.86                     | 0.75              |
| 4:AD:170:VAL:HG11  | 4:AD:174:LEU:HB2  | 1.68                     | 0.75              |
| 4:AD:58:LEU:O      | 4:AD:58:LEU:HD22  | 1.87                     | 0.75              |
| 12:AL:48:ALA:C     | 12:AL:49:LEU:HD22 | 2.06                     | 0.75              |
| 50:B1:29:GLY:O     | 50:B1:30:VAL:HG22 | 1.85                     | 0.75              |
| 27:BA:1400:G:H2'   | 27:BA:1401:G:H8   | 1.50                     | 0.75              |
| 27:BA:1890:A:H2'   | 27:BA:1891:G:O4'  | 1.86                     | 0.75              |
| 27:BA:2845:G:O2'   | 27:BA:2846:G:H5'  | 1.85                     | 0.75              |
| 34:BH:85:LYS:HE2   | 34:BH:145:ALA:HB2 | 1.67                     | 0.75              |
| 44:BV:19:LYS:HG3   | 44:BV:20:LEU:O    | 1.85                     | 0.75              |
| 1:CA:1355:G:H2'    | 1:CA:1356:G:H8    | 1.50                     | 0.75              |
| 1:CA:9:G:H5'       | 5:CE:122:GLU:OE1  | 1.86                     | 0.75              |
| 5:CE:53:LEU:HD12   | 5:CE:53:LEU:H     | 1.51                     | 0.75              |
| 18:CR:62:GLU:HA    | 18:CR:65:ILE:HD12 | 1.66                     | 0.75              |
| 18:CR:82:THR:CG2   | 18:CR:83:GLU:H    | 1.98                     | 0.75              |
| 27:DA:1215:G:H2'   | 27:DA:1216:G:O4'  | 1.86                     | 0.75              |
| 27:DA:2615:U:C2    | 54:D5:7:PRO:HA    | 2.21                     | 0.75              |
| 27:DA:760:G:O2'    | 27:DA:761:A:H5'   | 1.85                     | 0.75              |
| 27:DA:852:G:N2     | 27:DA:926:A:H1'   | 2.02                     | 0.75              |
| 30:DD:43:ARG:NH1   | 30:DD:44:ASN:ND2  | 2.34                     | 0.75              |
| 31:DE:1:MET:N      | 31:DE:84:PHE:HB2  | 2.01                     | 0.75              |
| 33:DG:45:GLU:H     | 33:DG:88:ILE:HD13 | 1.51                     | 0.75              |
| 42:DT:16:ARG:HB3   | 42:DT:19:LEU:HD11 | 1.67                     | 0.75              |
| 27:DA:560:C:H4'    | 43:DU:52:ARG:HH22 | 1.49                     | 0.75              |
| 43:DU:89:GLU:HG2   | 44:DV:50:PRO:HG3  | 1.69                     | 0.75              |
| 13:AM:96:LEU:CD2   | 13:AM:97:PRO:HD2  | 2.16                     | 0.75              |
| 16:AP:14:ASN:N     | 16:AP:15:PRO:HD3  | 2.01                     | 0.75              |
| 55:B6:19:ARG:HG2   | 55:B6:20:ASN:N    | 2.00                     | 0.75              |
| 38:BP:49:ARG:HD2   | 57:B8:59:LYS:HG2  | 1.69                     | 0.75              |
| 27:BA:339:U:O2'    | 27:BA:340:A:H5'   | 1.84                     | 0.75              |
| 27:BA:2810:A:H2'   | 31:BE:61:ARG:HH21 | 1.51                     | 0.75              |
| 33:BG:170:ARG:HD2  | 33:BG:174:GLU:HB2 | 1.68                     | 0.75              |
| 35:BI:123:LEU:HD21 | 35:BI:143:SER:O   | 1.87                     | 0.75              |
| 1:CA:1254:C:OP1    | 10:CJ:45:ARG:HA   | 1.86                     | 0.75              |
| 1:CA:184:G:H2'     | 1:CA:185:A:H8     | 1.50                     | 0.75              |
| 17:CQ:4:LYS:HE3    | 17:CQ:6:LEU:HD11  | 1.67                     | 0.75              |
| 23:CW:17:G:H1      | 23:CW:54:U:H1'    | 1.51                     | 0.75              |
| 27:DA:1822:G:O2'   | 27:DA:1823:G:H5'  | 1.86                     | 0.75              |
| 42:DT:62:THR:HA    | 42:DT:74:ARG:O    | 1.86                     | 0.75              |
| 47:DY:27:VAL:HG12  | 47:DY:28:LYS:N    | 2.01                     | 0.75              |
| 47:DY:29:GLU:N     | 47:DY:29:GLU:OE1  | 2.20                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:DY:96:ILE:HD12  | 47:DY:99:CYS:CB    | 2.17                     | 0.75              |
| 1:AA:1508:G:H2'    | 1:AA:1509:C:H6     | 1.51                     | 0.75              |
| 8:AH:101:PRO:HG2   | 8:AH:133:LEU:HD11  | 1.67                     | 0.75              |
| 15:AO:26:GLU:OE2   | 15:AO:77:ARG:HD2   | 1.86                     | 0.75              |
| 19:AS:24:ALA:O     | 19:AS:25:LYS:HB2   | 1.85                     | 0.75              |
| 25:AY:68:C:C2'     | 25:AY:69:C:H5''    | 2.16                     | 0.75              |
| 27:BA:1179:C:H2'   | 27:BA:1180:C:H5''  | 1.67                     | 0.75              |
| 27:BA:125:G:H21    | 56:B7:48:LYS:NZ    | 1.84                     | 0.75              |
| 27:BA:1843:C:H5'   | 30:BD:253:GLN:NE2  | 2.02                     | 0.75              |
| 27:BA:2571:C:H5'   | 27:BA:2572:A:C5'   | 2.16                     | 0.75              |
| 27:BA:2870:C:H2'   | 27:BA:2871:C:C5'   | 2.15                     | 0.75              |
| 27:BA:558:G:P      | 36:BN:111:PRO:HD2  | 2.26                     | 0.75              |
| 31:BE:167:VAL:HG23 | 31:BE:170:LEU:HD11 | 1.68                     | 0.75              |
| 47:BY:7:VAL:C      | 47:BY:8:LYS:HD2    | 2.06                     | 0.75              |
| 10:CJ:40:LEU:HG    | 10:CJ:69:ASN:HB3   | 1.68                     | 0.75              |
| 12:CL:73:ASN:ND2   | 12:CL:105:ALA:HB2  | 2.02                     | 0.75              |
| 27:DA:136:G:H1     | 27:DA:143(A):C:H42 | 1.33                     | 0.75              |
| 27:DA:1697:G:H3'   | 27:DA:1698:A:H5''  | 1.69                     | 0.75              |
| 27:DA:2564:A:C2    | 27:DA:2647:U:H4'   | 2.21                     | 0.75              |
| 27:DA:633:A:H2'    | 27:DA:634:C:C5'    | 2.14                     | 0.75              |
| 35:DI:83:ALA:HA    | 35:DI:89:TYR:CE1   | 2.22                     | 0.75              |
| 37:DO:6:THR:HG22   | 37:DO:7:TYR:H      | 1.51                     | 0.75              |
| 1:AA:1068:G:OP2    | 1:AA:1094:G:H5''   | 1.86                     | 0.75              |
| 1:AA:170:U:O2'     | 1:AA:171:A:H5'     | 1.86                     | 0.75              |
| 1:AA:441:A:H3'     | 1:AA:442:C:H6      | 1.49                     | 0.75              |
| 27:BA:2466:C:H5''  | 58:B9:6:SER:HB2    | 1.67                     | 0.75              |
| 30:BD:34:VAL:O     | 30:BD:34:VAL:HG13  | 1.87                     | 0.75              |
| 32:BF:63:LYS:HA    | 32:BF:76:GLY:O     | 1.87                     | 0.75              |
| 37:BO:16:ALA:HB2   | 37:BO:52:VAL:CG1   | 2.15                     | 0.75              |
| 38:BP:146:VAL:O    | 38:BP:148:LEU:HG   | 1.87                     | 0.75              |
| 40:BR:10:LEU:HA    | 40:BR:17:ARG:HD2   | 1.67                     | 0.75              |
| 43:BU:104:GLN:NE2  | 43:BU:105:VAL:HG23 | 1.98                     | 0.75              |
| 1:CA:821:G:H2'     | 1:CA:822:C:H6      | 1.51                     | 0.75              |
| 3:CC:92:ALA:HB2    | 3:CC:99:VAL:CG2    | 2.16                     | 0.75              |
| 21:CU:2:GLY:C      | 21:CU:4:GLY:H      | 1.90                     | 0.75              |
| 27:DA:1560:G:N2    | 27:DA:1561:G:H1'   | 2.02                     | 0.75              |
| 27:DA:1946:U:H2'   | 27:DA:1947:C:H6    | 1.52                     | 0.75              |
| 27:DA:2547:U:H2'   | 27:DA:2548:G:C8    | 2.21                     | 0.75              |
| 32:DF:187:VAL:CG1  | 38:DP:7:ARG:HH21   | 1.99                     | 0.75              |
| 32:DF:22:ALA:C     | 32:DF:24:LEU:H     | 1.87                     | 0.75              |
| 37:DO:87:ILE:HD11  | 37:DO:114:ILE:HD11 | 1.67                     | 0.75              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1285:A:H5'   | 1:AA:1286:A:C8     | 2.21                     | 0.75              |
| 1:AA:687:A:N3     | 1:AA:688:G:H1'     | 2.00                     | 0.75              |
| 4:AD:146:ILE:HD12 | 4:AD:146:ILE:H     | 1.50                     | 0.75              |
| 25:AY:30:A:H2'    | 25:AY:31:U:H6      | 1.50                     | 0.75              |
| 50:B1:19:GLN:HB2  | 50:B1:36:GLY:H     | 1.52                     | 0.75              |
| 27:BA:1289:C:H5'  | 27:BA:1289:C:H6    | 1.51                     | 0.75              |
| 27:BA:2114:A:H2'  | 27:BA:2115:G:O4'   | 1.87                     | 0.75              |
| 27:BA:549:G:H2'   | 27:BA:551:G:H5''   | 1.66                     | 0.75              |
| 30:BD:143:HIS:ND1 | 30:BD:194:GLY:O    | 2.19                     | 0.75              |
| 32:BF:20:LEU:HD22 | 32:BF:203:GLN:NE2  | 2.01                     | 0.75              |
| 41:BS:36:TYR:CD2  | 41:BS:52:SER:HB2   | 2.20                     | 0.75              |
| 1:CA:999:C:O2'    | 1:CA:1000:U:H5'    | 1.87                     | 0.75              |
| 1:CA:840:C:H5''   | 1:CA:841:U:OP1     | 1.87                     | 0.75              |
| 2:CB:27:LYS:HB2   | 2:CB:193:ASP:HB2   | 1.68                     | 0.75              |
| 3:CC:39:ILE:HG22  | 3:CC:43:LEU:HD12   | 1.68                     | 0.75              |
| 10:CJ:40:LEU:HB2  | 10:CJ:41:PRO:HD2   | 1.69                     | 0.75              |
| 11:CK:17:GLY:HA3  | 11:CK:77:MET:SD    | 2.26                     | 0.75              |
| 1:CA:1313:U:OP1   | 19:CS:6:LYS:HG3    | 1.87                     | 0.75              |
| 51:D2:12:GLU:O    | 51:D2:16:LEU:HG    | 1.86                     | 0.75              |
| 57:D8:11:LYS:HE2  | 57:D8:64:TYR:HE1   | 1.51                     | 0.75              |
| 27:DA:1590:U:H2'  | 27:DA:1591:G:H5''  | 1.68                     | 0.75              |
| 27:DA:1947:C:H42  | 27:DA:1959:G:H1    | 1.35                     | 0.75              |
| 27:DA:2887:U:H2'  | 27:DA:2888:C:C6    | 2.20                     | 0.75              |
| 27:DA:520:G:H2'   | 27:DA:521:G:C8     | 2.22                     | 0.75              |
| 27:DA:649:G:H2'   | 27:DA:650:C:C6     | 2.22                     | 0.75              |
| 27:DA:851:U:H3    | 27:DA:926:A:H61    | 1.33                     | 0.75              |
| 27:DA:979:G:N2    | 27:DA:985:C:H42    | 1.85                     | 0.75              |
| 33:DG:77:ILE:H    | 33:DG:83:ARG:HB3   | 1.51                     | 0.75              |
| 34:DH:144:VAL:O   | 34:DH:148:ILE:HG12 | 1.86                     | 0.75              |
| 27:DA:908:C:H3'   | 39:DQ:22:LYS:HZ1   | 1.51                     | 0.75              |
| 4:AD:98:GLU:HG3   | 4:AD:103:ASN:ND2   | 2.01                     | 0.75              |
| 17:AQ:74:LEU:HD13 | 17:AQ:74:LEU:O     | 1.86                     | 0.75              |
| 18:AR:43:PHE:O    | 18:AR:51:LEU:HD12  | 1.87                     | 0.75              |
| 27:BA:176:G:O2'   | 27:BA:177:G:H5'    | 1.85                     | 0.75              |
| 27:BA:514:A:H1'   | 27:BA:581:C:O2'    | 1.87                     | 0.75              |
| 36:BN:93:THR:HG23 | 36:BN:93:THR:O     | 1.86                     | 0.75              |
| 3:CC:40:ARG:HB3   | 3:CC:44:GLU:OE2    | 1.87                     | 0.75              |
| 4:CD:146:ILE:HD12 | 4:CD:146:ILE:N     | 2.02                     | 0.75              |
| 5:CE:15:ARG:HG3   | 5:CE:28:PHE:CE2    | 2.21                     | 0.75              |
| 7:CG:78:ARG:CG    | 7:CG:79:ARG:H      | 1.99                     | 0.75              |
| 8:CH:72:PRO:O     | 8:CH:73:ASP:HB3    | 1.85                     | 0.75              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:CJ:12:ASP:OD1   | 10:CJ:15:THR:HG23   | 1.86                     | 0.75              |
| 27:DA:1416:G:O2'   | 27:DA:1417:C:H6     | 1.68                     | 0.75              |
| 27:DA:271(M):G:H2' | 27:DA:271(N):U:H5'' | 1.69                     | 0.75              |
| 27:DA:800:A:H1'    | 27:DA:802:A:OP2     | 1.86                     | 0.75              |
| 29:DC:77:ILE:HG21  | 29:DC:123:VAL:H     | 1.52                     | 0.75              |
| 37:DO:87:ILE:HG21  | 37:DO:91:LEU:HA     | 1.69                     | 0.75              |
| 39:DQ:85:LYS:CG    | 49:D0:7:LEU:HD13    | 2.16                     | 0.75              |
| 40:DR:11:ASN:HB3   | 40:DR:12:ARG:NH1    | 2.01                     | 0.75              |
| 1:AA:1239:A:H62    | 1:AA:1299:A:H62     | 1.33                     | 0.75              |
| 6:AF:75:LEU:HD23   | 6:AF:79:LEU:HG      | 1.68                     | 0.75              |
| 27:BA:271(U):G:O2' | 27:BA:271(V):G:H5'  | 1.87                     | 0.75              |
| 27:BA:703:U:C2'    | 27:BA:704:G:H5'     | 2.16                     | 0.75              |
| 27:BA:71:A:H3'     | 27:BA:71:A:OP2      | 1.86                     | 0.75              |
| 30:BD:118:VAL:HG22 | 30:BD:119:ALA:N     | 1.97                     | 0.75              |
| 34:BH:44:VAL:HG12  | 34:BH:45:VAL:N      | 1.97                     | 0.75              |
| 35:BI:115:ALA:CB   | 35:BI:129:THR:H     | 1.98                     | 0.75              |
| 38:BP:23:PRO:HD2   | 38:BP:33:ARG:NH2    | 2.01                     | 0.75              |
| 27:BA:2875:C:O2'   | 42:BT:5:ALA:CB      | 2.35                     | 0.75              |
| 27:BA:559:G:H22    | 43:BU:49:HIS:CD2    | 2.05                     | 0.75              |
| 43:BU:8:VAL:HG11   | 43:BU:12:ARG:NE     | 2.01                     | 0.75              |
| 55:D6:33:LYS:HA    | 55:D6:33:LYS:CE     | 2.05                     | 0.75              |
| 58:D9:4:ARG:O      | 58:D9:36:GLN:HA     | 1.87                     | 0.75              |
| 27:DA:2283:C:H2'   | 27:DA:2284:C:H5'    | 1.68                     | 0.75              |
| 27:DA:2756:U:H4'   | 27:DA:2757:A:O5'    | 1.85                     | 0.75              |
| 33:DG:161:THR:HG22 | 33:DG:163:ALA:H     | 1.50                     | 0.75              |
| 36:DN:58:ASP:O     | 36:DN:60:ILE:N      | 2.18                     | 0.75              |
| 38:DP:48:PRO:CG    | 38:DP:49:ARG:H      | 1.99                     | 0.75              |
| 42:DT:28:VAL:HB    | 42:DT:88:ILE:HG12   | 1.68                     | 0.75              |
| 1:AA:992:U:H3      | 1:AA:1044:A:H62     | 1.33                     | 0.75              |
| 5:AE:76:ILE:HD11   | 5:AE:142:LEU:HD21   | 1.68                     | 0.75              |
| 11:AK:61:ALA:O     | 11:AK:64:ALA:HB3    | 1.85                     | 0.75              |
| 27:BA:1273:U:H6    | 27:BA:1273:U:C5'    | 2.00                     | 0.75              |
| 48:BZ:152:SER:H    | 48:BZ:166:PRO:HB3   | 1.51                     | 0.75              |
| 1:CA:1285:A:O2'    | 1:CA:1286:A:OP2     | 2.04                     | 0.75              |
| 19:CS:19:VAL:CG1   | 19:CS:44:MET:HG3    | 2.14                     | 0.75              |
| 21:CU:24:ARG:O     | 21:CU:25:LYS:HB2    | 1.85                     | 0.75              |
| 25:CY:57:A:H2'     | 25:CY:60:C:H41      | 1.52                     | 0.75              |
| 27:DA:140:G:HO2'   | 27:DA:141:A:H2      | 1.35                     | 0.75              |
| 27:DA:1968:G:C2'   | 27:DA:1969:A:H5''   | 2.15                     | 0.75              |
| 34:DH:147:ASN:N    | 34:DH:147:ASN:HD22  | 1.85                     | 0.75              |
| 35:DI:37:VAL:CG1   | 35:DI:38:LEU:HD12   | 2.16                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DI:81:VAL:HG12  | 35:DI:82:ARG:H     | 1.51                     | 0.75              |
| 36:DN:70:LYS:HB3   | 36:DN:87:LEU:HB2   | 1.69                     | 0.75              |
| 37:DO:35:VAL:HG21  | 37:DO:69:ILE:CD1   | 2.17                     | 0.75              |
| 1:AA:1406:U:H2'    | 1:AA:1407:C:H5'    | 1.69                     | 0.74              |
| 1:AA:9:G:OP1       | 5:AE:122:GLU:HG3   | 1.86                     | 0.74              |
| 20:AT:63:ILE:HD13  | 20:AT:80:ARG:HB2   | 1.69                     | 0.74              |
| 51:B2:4:SER:O      | 51:B2:7:ARG:HG2    | 1.86                     | 0.74              |
| 27:BA:1033:U:H5''  | 27:BA:1034:G:OP1   | 1.87                     | 0.74              |
| 27:BA:748:G:C8     | 45:BW:89:ALA:HB1   | 2.21                     | 0.74              |
| 30:BD:137:PRO:O    | 30:BD:140:THR:HG23 | 1.85                     | 0.74              |
| 39:BQ:106:VAL:HG21 | 39:BQ:114:ALA:HB1  | 1.67                     | 0.74              |
| 40:BR:24:GLN:NE2   | 40:BR:36:THR:HG21  | 2.02                     | 0.74              |
| 43:BU:29:SER:O     | 43:BU:30:LYS:HD3   | 1.87                     | 0.74              |
| 1:CA:386:C:H2'     | 1:CA:387:U:C5'     | 2.17                     | 0.74              |
| 13:CM:30:ALA:O     | 13:CM:34:LEU:HG    | 1.86                     | 0.74              |
| 20:CT:48:LYS:O     | 20:CT:49:ALA:HB2   | 1.87                     | 0.74              |
| 23:CW:53:U:H4'     | 39:DQ:52:VAL:HG22  | 1.69                     | 0.74              |
| 25:CY:68:C:C2'     | 25:CY:69:C:H5''    | 2.17                     | 0.74              |
| 52:D3:7:LYS:HG2    | 52:D3:8:LEU:H      | 1.50                     | 0.74              |
| 27:DA:2509:G:H2'   | 27:DA:2510:C:H6    | 1.52                     | 0.74              |
| 27:DA:2550:G:C2'   | 27:DA:2551:C:H5'   | 2.17                     | 0.74              |
| 27:DA:2560:C:N4    | 27:DA:2561:A:H62   | 1.84                     | 0.74              |
| 27:DA:55:G:H2'     | 27:DA:56:A:H8      | 1.50                     | 0.74              |
| 27:DA:820:A:H2'    | 27:DA:821:A:O4'    | 1.86                     | 0.74              |
| 30:DD:239:ARG:NH2  | 30:DD:239:ARG:HG2  | 1.88                     | 0.74              |
| 32:DF:126:VAL:O    | 32:DF:196:LEU:HG   | 1.87                     | 0.74              |
| 33:DG:114:ILE:HG12 | 33:DG:140:ILE:HD13 | 1.68                     | 0.74              |
| 34:DH:17:VAL:HB    | 34:DH:45:VAL:HG13  | 1.69                     | 0.74              |
| 34:DH:85:LYS:HB3   | 34:DH:133:VAL:O    | 1.87                     | 0.74              |
| 35:DI:133:HIS:HB2  | 35:DI:134:PRO:CD   | 2.16                     | 0.74              |
| 37:DO:1:MET:HG3    | 37:DO:32:TYR:CD1   | 2.22                     | 0.74              |
| 37:DO:87:ILE:HG22  | 37:DO:88:ASN:O     | 1.87                     | 0.74              |
| 38:DP:33:ARG:O     | 38:DP:34:GLY:C     | 2.25                     | 0.74              |
| 41:DS:89:ARG:HB3   | 41:DS:92:TYR:HB2   | 1.69                     | 0.74              |
| 42:DT:105:LEU:HB3  | 42:DT:109:GLU:OE1  | 1.86                     | 0.74              |
| 1:AA:943:U:H1'     | 9:AI:124:GLN:HE22  | 1.52                     | 0.74              |
| 16:AP:21:VAL:CG1   | 16:AP:33:ILE:HB    | 2.17                     | 0.74              |
| 27:BA:71:A:C8      | 27:BA:71:A:H5'     | 2.21                     | 0.74              |
| 33:BG:51:ARG:NE    | 33:BG:51:ARG:HA    | 2.00                     | 0.74              |
| 43:BU:83:LEU:HG    | 43:BU:88:ILE:HG13  | 1.70                     | 0.74              |
| 48:BZ:102:ARG:HD3  | 48:BZ:135:PHE:CE1  | 2.22                     | 0.74              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1073:U:H2'    | 1:CA:1074:G:H8    | 1.52                     | 0.74              |
| 1:CA:939:G:H5''    | 7:CG:102:ARG:HH12 | 1.52                     | 0.74              |
| 55:D6:15:GLU:HG2   | 55:D6:18:ARG:HE   | 1.51                     | 0.74              |
| 27:DA:1468:C:H2'   | 27:DA:1469:A:H8   | 1.52                     | 0.74              |
| 27:DA:2384:G:H5''  | 27:DA:2386:C:OP1  | 1.87                     | 0.74              |
| 27:DA:265:A:H1'    | 27:DA:266:G:O4'   | 1.86                     | 0.74              |
| 39:DQ:44:ALA:HB3   | 39:DQ:45:GLN:HE21 | 1.50                     | 0.74              |
| 42:DT:35:LYS:NZ    | 42:DT:41:ARG:HE   | 1.86                     | 0.74              |
| 46:DX:64:LYS:HZ2   | 46:DX:73:ARG:HH12 | 1.34                     | 0.74              |
| 1:AA:1408:A:O2'    | 1:AA:1409:C:H5'   | 1.87                     | 0.74              |
| 2:AB:61:LEU:CD2    | 2:AB:68:ILE:HD11  | 2.17                     | 0.74              |
| 4:AD:105:VAL:HG13  | 4:AD:110:PHE:CD2  | 2.21                     | 0.74              |
| 4:AD:8:VAL:HB      | 4:AD:22:LYS:NZ    | 2.03                     | 0.74              |
| 5:AE:11:ILE:HG21   | 5:AE:105:VAL:HG22 | 1.67                     | 0.74              |
| 6:AF:16:GLN:NE2    | 6:AF:16:GLN:N     | 2.34                     | 0.74              |
| 12:AL:80:VAL:HA    | 12:AL:102:TYR:HD1 | 1.51                     | 0.74              |
| 15:AO:33:THR:HG23  | 15:AO:63:ARG:HH11 | 1.52                     | 0.74              |
| 1:AA:323:U:O3'     | 20:AT:22:ARG:HD3  | 1.86                     | 0.74              |
| 23:AW:10:G:N2      | 23:AW:25:A:H1'    | 2.02                     | 0.74              |
| 27:BA:1441:G:H2'   | 27:BA:1442:G:H8   | 1.51                     | 0.74              |
| 27:BA:1643:G:N2    | 27:BA:1644:C:H1'  | 2.01                     | 0.74              |
| 27:BA:2052:G:H4'   | 31:BE:143:ASN:O   | 1.87                     | 0.74              |
| 27:BA:485:C:H2'    | 27:BA:486:C:C6    | 2.22                     | 0.74              |
| 27:BA:648:G:H2'    | 27:BA:649:G:C8    | 2.21                     | 0.74              |
| 27:BA:676:A:H2     | 27:BA:802:A:H61   | 1.33                     | 0.74              |
| 28:BB:91:C:H2'     | 28:BB:92:C:C6     | 2.23                     | 0.74              |
| 34:BH:45:VAL:O     | 34:BH:45:VAL:HG12 | 1.87                     | 0.74              |
| 38:BP:126:VAL:HA   | 38:BP:145:PRO:HB2 | 1.66                     | 0.74              |
| 40:BR:100:LEU:HD21 | 40:BR:113:LEU:CD1 | 2.13                     | 0.74              |
| 47:BY:29:GLU:N     | 47:BY:29:GLU:OE1  | 2.20                     | 0.74              |
| 1:CA:1154:G:O2'    | 1:CA:1155:G:H8    | 1.68                     | 0.74              |
| 1:CA:1191:A:H5''   | 3:CC:4:LYS:NZ     | 2.02                     | 0.74              |
| 27:DA:1157:G:H2'   | 27:DA:1158:C:C6   | 2.22                     | 0.74              |
| 27:DA:533:G:O2'    | 43:DU:42:ALA:HB2  | 1.88                     | 0.74              |
| 27:DA:962:G:O2'    | 27:DA:963:U:H5'   | 1.85                     | 0.74              |
| 27:DA:993:G:O2'    | 27:DA:994:C:H5'   | 1.87                     | 0.74              |
| 28:DB:20:C:C2'     | 28:DB:21:G:H5'    | 2.17                     | 0.74              |
| 30:DD:72:LYS:HE2   | 30:DD:101:GLU:OE2 | 1.87                     | 0.74              |
| 30:DD:30:GLU:HA    | 30:DD:83:GLU:OE1  | 1.87                     | 0.74              |
| 33:DG:111:LEU:HD22 | 33:DG:117:PHE:CZ  | 2.22                     | 0.74              |
| 37:DO:18:LYS:HB2   | 37:DO:45:GLU:HG2  | 1.69                     | 0.74              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:DU:74:LEU:O     | 43:DU:74:LEU:HD12 | 1.88                     | 0.74              |
| 47:DY:28:LYS:N     | 47:DY:28:LYS:HZ2  | 1.84                     | 0.74              |
| 1:AA:1464:G:O2'    | 1:AA:1465:C:H5'   | 1.87                     | 0.74              |
| 2:AB:69:LEU:CD2    | 2:AB:159:PRO:HG2  | 2.18                     | 0.74              |
| 2:AB:68:ILE:HD12   | 2:AB:161:ALA:HB3  | 1.69                     | 0.74              |
| 27:BA:151:C:O2'    | 27:BA:152:G:H5'   | 1.87                     | 0.74              |
| 27:BA:2580:U:H5'   | 31:BE:131:ALA:HB2 | 1.68                     | 0.74              |
| 27:BA:2834:G:H5'   | 27:BA:2835:A:OP2  | 1.87                     | 0.74              |
| 27:BA:406:G:H8     | 27:BA:406:G:O5'   | 1.70                     | 0.74              |
| 1:CA:20:U:H2'      | 1:CA:21:G:O4'     | 1.87                     | 0.74              |
| 1:CA:259:G:O2'     | 1:CA:260:G:H5'    | 1.87                     | 0.74              |
| 1:CA:425:G:O2'     | 1:CA:426:G:H5'    | 1.86                     | 0.74              |
| 5:CE:105:VAL:O     | 5:CE:108:ALA:HB3  | 1.87                     | 0.74              |
| 10:CJ:22:LYS:NZ    | 10:CJ:23:ILE:HG12 | 2.03                     | 0.74              |
| 11:CK:21:ILE:HD11  | 11:CK:82:VAL:HG13 | 1.68                     | 0.74              |
| 27:DA:2815:C:H2'   | 27:DA:2816:C:H6   | 1.51                     | 0.74              |
| 28:DB:22:U:H3      | 28:DB:61:G:H1     | 1.35                     | 0.74              |
| 1:AA:1397:C:H3'    | 1:AA:1398:A:H5'   | 1.66                     | 0.74              |
| 6:AF:18:GLN:HA     | 6:AF:21:LEU:HB2   | 1.69                     | 0.74              |
| 7:AG:28:ASN:HA     | 7:AG:31:MET:HE2   | 1.68                     | 0.74              |
| 27:BA:1848:A:HO2'  | 27:BA:1849:G:H8   | 1.31                     | 0.74              |
| 27:BA:1929:G:H4'   | 27:BA:1930:G:OP1  | 1.86                     | 0.74              |
| 27:BA:2412:A:H2'   | 27:BA:2413:G:O4'  | 1.87                     | 0.74              |
| 27:BA:2516:G:H2'   | 27:BA:2517:C:H5'  | 1.70                     | 0.74              |
| 30:BD:64:ILE:HG23  | 30:BD:64:ILE:O    | 1.87                     | 0.74              |
| 31:BE:9:VAL:HG12   | 31:BE:25:VAL:O    | 1.88                     | 0.74              |
| 36:BN:32:THR:HG22  | 36:BN:37:LYS:HB3  | 1.67                     | 0.74              |
| 37:BO:110:GLY:HA2  | 37:BO:112:MET:HE3 | 1.68                     | 0.74              |
| 4:CD:33:MET:CE     | 4:CD:37:PRO:HA    | 2.17                     | 0.74              |
| 12:CL:25:LYS:NZ    | 12:CL:30:ARG:HH22 | 1.85                     | 0.74              |
| 27:DA:133:C:H42    | 27:DA:146:G:H1    | 0.83                     | 0.74              |
| 27:DA:1495:A:H2'   | 27:DA:1496:A:C2   | 2.23                     | 0.74              |
| 29:DC:78:ALA:HB2   | 29:DC:82:LYS:HD2  | 1.69                     | 0.74              |
| 37:DO:35:VAL:HG22  | 37:DO:65:THR:CG2  | 2.17                     | 0.74              |
| 38:DP:106:LEU:HD11 | 38:DP:112:LEU:HB2 | 1.69                     | 0.74              |
| 2:AB:21:ARG:HB2    | 2:AB:38:GLY:O     | 1.86                     | 0.74              |
| 5:AE:72:GLN:HE21   | 5:AE:144:THR:HG22 | 1.52                     | 0.74              |
| 14:AN:13:THR:N     | 14:AN:14:PRO:HD2  | 2.02                     | 0.74              |
| 27:BA:591:C:O2     | 57:B8:2:PRO:HA    | 1.87                     | 0.74              |
| 27:BA:634:C:H2'    | 27:BA:635:C:C6    | 2.22                     | 0.74              |
| 27:BA:71:A:H5''    | 27:BA:73:A:C8     | 2.23                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:847:U:H2'   | 27:BA:848:G:H5''   | 1.69                     | 0.74              |
| 30:BD:31:LYS:HB3  | 30:BD:35:LYS:HG3   | 1.68                     | 0.74              |
| 30:BD:60:ARG:HD3  | 30:BD:86:PRO:CB    | 2.16                     | 0.74              |
| 31:BE:40:GLU:N    | 31:BE:40:GLU:OE1   | 2.21                     | 0.74              |
| 44:BV:34:GLU:HG2  | 44:BV:36:PRO:HD3   | 1.69                     | 0.74              |
| 27:BA:64:A:C4     | 46:BX:66:LEU:HD12  | 2.22                     | 0.74              |
| 27:DA:66:C:H2'    | 27:DA:67:U:C6      | 2.22                     | 0.74              |
| 31:DE:116:VAL:O   | 31:DE:117:MET:CB   | 2.33                     | 0.74              |
| 35:DI:83:ALA:CB   | 35:DI:88:ILE:HA    | 2.17                     | 0.74              |
| 2:AB:114:ARG:HA   | 2:AB:117:GLU:HB2   | 1.69                     | 0.74              |
| 6:AF:10:LEU:HD12  | 6:AF:10:LEU:N      | 2.02                     | 0.74              |
| 10:AJ:63:PHE:HB3  | 14:AN:58:LYS:HA    | 1.69                     | 0.74              |
| 13:AM:57:ARG:CZ   | 53:B4:60:GLU:HG3   | 2.18                     | 0.74              |
| 51:B2:33:MET:C    | 51:B2:35:LEU:H     | 1.91                     | 0.74              |
| 55:B6:41:PRO:HD3  | 55:B6:46:HIS:HB3   | 1.68                     | 0.74              |
| 27:BA:1322:A:H2'  | 27:BA:1323:U:H6    | 1.51                     | 0.74              |
| 27:BA:2415:G:H4'  | 38:BP:66:GLY:HA3   | 1.67                     | 0.74              |
| 27:BA:2533:A:H2'  | 27:BA:2534:A:H5''  | 1.70                     | 0.74              |
| 34:BH:138:LYS:H   | 34:BH:141:VAL:HG23 | 1.51                     | 0.74              |
| 45:BW:15:ARG:HA   | 45:BW:18:ARG:HD2   | 1.69                     | 0.74              |
| 45:BW:81:ALA:O    | 45:BW:82:LEU:HD23  | 1.88                     | 0.74              |
| 1:CA:237:C:H5''   | 17:CQ:25:ARG:NH1   | 2.02                     | 0.74              |
| 1:CA:256:U:H2'    | 1:CA:257:G:H8      | 1.50                     | 0.74              |
| 1:CA:971:G:H5''   | 1:CA:972:C:H5''    | 1.69                     | 0.74              |
| 2:CB:36:ARG:NE    | 2:CB:36:ARG:HA     | 2.02                     | 0.74              |
| 8:CH:104:ARG:CB   | 8:CH:108:GLY:H     | 2.01                     | 0.74              |
| 12:CL:67:ILE:HD13 | 12:CL:74:LEU:HD12  | 1.68                     | 0.74              |
| 13:CM:51:ALA:O    | 13:CM:55:ARG:HB3   | 1.87                     | 0.74              |
| 13:CM:66:LEU:O    | 13:CM:67:GLU:O     | 2.06                     | 0.74              |
| 27:DA:1014:U:H2'  | 27:DA:1015:G:C8    | 2.22                     | 0.74              |
| 27:DA:2181:G:O2'  | 27:DA:2182:G:H5'   | 1.88                     | 0.74              |
| 27:DA:2312:U:H2'  | 27:DA:2313:C:H5''  | 1.70                     | 0.74              |
| 27:DA:2836:U:H2'  | 27:DA:2837:G:C8    | 2.22                     | 0.74              |
| 27:DA:411:G:N2    | 38:DP:71:VAL:HG21  | 2.02                     | 0.74              |
| 28:DB:28:C:O2'    | 28:DB:29:A:H5'     | 1.87                     | 0.74              |
| 27:DA:1567:A:H5'' | 30:DD:58:HIS:CD2   | 2.23                     | 0.74              |
| 31:DE:117:MET:O   | 31:DE:118:LYS:HB2  | 1.86                     | 0.74              |
| 32:DF:57:VAL:CG1  | 32:DF:59:TYR:CD1   | 2.71                     | 0.74              |
| 36:DN:18:ALA:HB1  | 36:DN:21:LYS:HB2   | 1.68                     | 0.74              |
| 39:DQ:42:ILE:H    | 39:DQ:42:ILE:HD12  | 1.52                     | 0.74              |
| 1:AA:21:G:H2'     | 1:AA:22:G:C8       | 2.23                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:531:U:H5''    | 1:AA:532:A:OP1     | 1.87                     | 0.74              |
| 1:AA:979:C:C3'     | 1:AA:980:C:H5''    | 2.17                     | 0.74              |
| 8:AH:35:ILE:O      | 8:AH:39:LEU:HD23   | 1.88                     | 0.74              |
| 9:AI:95:LYS:O      | 9:AI:99:LEU:HB2    | 1.87                     | 0.74              |
| 11:AK:79:SER:HB2   | 11:AK:106:LYS:HE2  | 1.69                     | 0.74              |
| 51:B2:53:LEU:HD22  | 51:B2:57:ILE:HD11  | 1.69                     | 0.74              |
| 53:B4:53:THR:O     | 53:B4:54:LYS:HG2   | 1.85                     | 0.74              |
| 28:BB:88:C:H2'     | 28:BB:89:G:C8      | 2.23                     | 0.74              |
| 32:BF:164:ARG:HH11 | 32:BF:164:ARG:HG2  | 1.52                     | 0.74              |
| 35:BI:133:HIS:HB2  | 35:BI:134:PRO:HD2  | 1.70                     | 0.74              |
| 44:BV:47:VAL:HB    | 44:BV:49:THR:O     | 1.88                     | 0.74              |
| 1:CA:1141:C:H2'    | 1:CA:1142:G:C8     | 2.23                     | 0.74              |
| 1:CA:985:C:HO2'    | 1:CA:986:A:H8      | 1.36                     | 0.74              |
| 27:DA:15:G:OP1     | 54:D5:24:ALA:HB2   | 1.87                     | 0.74              |
| 27:DA:1225:G:OP1   | 44:DV:86:GLY:HA3   | 1.88                     | 0.74              |
| 27:DA:1400:G:H2'   | 27:DA:1401:G:H8    | 1.52                     | 0.74              |
| 27:DA:2339:G:O2'   | 27:DA:2340:G:H5'   | 1.88                     | 0.74              |
| 42:DT:88:ILE:HG22  | 42:DT:89:VAL:HG23  | 1.68                     | 0.74              |
| 48:DZ:150:HIS:CB   | 48:DZ:169:THR:HG22 | 2.18                     | 0.74              |
| 5:AE:129:ILE:CG2   | 5:AE:130:ASN:H     | 1.95                     | 0.74              |
| 8:AH:103:VAL:CG2   | 8:AH:110:ALA:HB2   | 2.17                     | 0.74              |
| 8:AH:110:ALA:HB3   | 8:AH:121:ASP:HB3   | 1.70                     | 0.74              |
| 27:BA:1447:G:H2'   | 27:BA:1448:G:H8    | 1.53                     | 0.74              |
| 27:BA:986:C:O2'    | 27:BA:987:G:H5'    | 1.88                     | 0.74              |
| 27:BA:1902:C:O2'   | 30:BD:244:ARG:HB2  | 1.88                     | 0.74              |
| 30:BD:35:LYS:HZ3   | 30:BD:103:ARG:CA   | 1.99                     | 0.74              |
| 34:BH:20:ALA:HB3   | 34:BH:23:ARG:HB2   | 1.70                     | 0.74              |
| 35:BI:129:THR:HG22 | 35:BI:137:PRO:HG3  | 1.69                     | 0.74              |
| 35:BI:77:LEU:HD23  | 35:BI:78:THR:H     | 1.51                     | 0.74              |
| 1:CA:1471:G:O2'    | 1:CA:1472:U:H5'    | 1.87                     | 0.74              |
| 27:DA:2426:A:H3'   | 27:DA:2427:C:C5'   | 2.18                     | 0.74              |
| 31:DE:51:PHE:CE1   | 31:DE:52:LEU:HD13  | 2.22                     | 0.74              |
| 37:DO:101:PRO:HG3  | 42:DT:67:SER:OG    | 1.88                     | 0.74              |
| 38:DP:102:ARG:HG2  | 38:DP:102:ARG:O    | 1.87                     | 0.74              |
| 42:DT:28:VAL:HG13  | 42:DT:46:GLU:HA    | 1.69                     | 0.74              |
| 1:AA:954:G:H21     | 1:AA:1227:A:H62    | 1.36                     | 0.74              |
| 3:AC:53:ALA:HB2    | 3:AC:115:LEU:HG    | 1.69                     | 0.74              |
| 13:AM:104:ARG:CG   | 13:AM:105:THR:H    | 2.01                     | 0.74              |
| 19:AS:44:MET:O     | 19:AS:47:HIS:HB2   | 1.88                     | 0.74              |
| 23:AW:22:G:H2'     | 23:AW:23:G:H5'     | 1.68                     | 0.74              |
| 55:B6:33:LYS:HA    | 55:B6:33:LYS:HE2   | 1.69                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:B8:23:VAL:HG12  | 57:B8:46:ARG:HB3   | 1.70                     | 0.74              |
| 27:BA:1557:C:OP2   | 27:BA:1558:A:H2'   | 1.87                     | 0.74              |
| 27:BA:2298:A:C2    | 27:BA:2299:G:H1'   | 2.23                     | 0.74              |
| 27:BA:356:G:H5'    | 27:BA:357:A:OP2    | 1.88                     | 0.74              |
| 30:BD:36:PRO:HB2   | 30:BD:61:LEU:HD11  | 1.70                     | 0.74              |
| 46:BX:12:VAL:HB    | 46:BX:17:ALA:CB    | 2.17                     | 0.74              |
| 1:CA:1479:C:O2'    | 1:CA:1480:G:H5'    | 1.88                     | 0.74              |
| 1:CA:93:G:C2'      | 1:CA:96:U:H5'      | 2.16                     | 0.74              |
| 2:CB:96:ARG:H      | 2:CB:96:ARG:CD     | 2.01                     | 0.74              |
| 5:CE:101:ILE:N     | 5:CE:101:ILE:HD13  | 2.03                     | 0.74              |
| 13:CM:14:ARG:H     | 13:CM:44:ARG:NH1   | 1.84                     | 0.74              |
| 13:CM:88:ARG:HA    | 13:CM:98:VAL:CG1   | 2.17                     | 0.74              |
| 15:CO:7:GLU:O      | 15:CO:11:VAL:HG23  | 1.88                     | 0.74              |
| 25:CY:40:C:H2'     | 25:CY:41:G:H8      | 1.51                     | 0.74              |
| 27:DA:514:A:C2'    | 27:DA:515:A:H5'    | 2.18                     | 0.74              |
| 40:DR:26:LYS:HE2   | 40:DR:71:GLN:H     | 1.52                     | 0.74              |
| 46:DX:61:GLY:HA3   | 46:DX:73:ARG:O     | 1.88                     | 0.74              |
| 1:AA:1360:A:O2'    | 1:AA:1361:G:H5'    | 1.88                     | 0.73              |
| 1:AA:179:A:H2'     | 1:AA:180:U:C6      | 2.23                     | 0.73              |
| 1:AA:942:G:H21     | 9:AI:124:GLN:NE2   | 1.85                     | 0.73              |
| 3:AC:141:VAL:HG11  | 3:AC:149:ALA:HB2   | 1.70                     | 0.73              |
| 4:AD:9:CYS:SG      | 60:AD:302:ZN:ZN    | 1.77                     | 0.73              |
| 5:AE:141:GLN:HG2   | 5:AE:143:ARG:HH22  | 1.53                     | 0.73              |
| 27:BA:1192:G:C2'   | 27:BA:1193:G:H5''  | 2.18                     | 0.73              |
| 27:BA:344:G:H22    | 27:BA:345:A:H62    | 1.32                     | 0.73              |
| 27:BA:673:C:H2'    | 27:BA:674:G:H5'    | 1.70                     | 0.73              |
| 30:BD:35:LYS:H     | 30:BD:36:PRO:HD2   | 1.53                     | 0.73              |
| 32:BF:20:LEU:HB3   | 32:BF:23:ASP:OD1   | 1.88                     | 0.73              |
| 1:CA:386:C:O2'     | 1:CA:387:U:H5'     | 1.88                     | 0.73              |
| 4:CD:82:ALA:CB     | 4:CD:89:THR:HG23   | 2.16                     | 0.73              |
| 15:CO:82:ILE:HG12  | 15:CO:87:ILE:HB    | 1.68                     | 0.73              |
| 19:CS:32:LYS:HE3   | 19:CS:32:LYS:N     | 2.03                     | 0.73              |
| 27:DA:1022:G:O6    | 36:DN:66:LYS:HE2   | 1.87                     | 0.73              |
| 27:DA:1991:U:O2'   | 27:DA:1992:G:H5''  | 1.87                     | 0.73              |
| 27:DA:271(H):G:H2' | 27:DA:271(I):G:C8  | 2.22                     | 0.73              |
| 27:DA:340:A:H2'    | 27:DA:341:G:O4'    | 1.87                     | 0.73              |
| 27:DA:36:G:H4'     | 27:DA:451:C:C2     | 2.23                     | 0.73              |
| 31:DE:34:VAL:O     | 31:DE:35:GLN:HB2   | 1.87                     | 0.73              |
| 33:DG:131:TYR:HE2  | 33:DG:133:LEU:HD23 | 1.53                     | 0.73              |
| 36:DN:13:TRP:O     | 36:DN:135:PRO:HD2  | 1.88                     | 0.73              |
| 36:DN:67:LEU:HB3   | 36:DN:88:GLU:HG2   | 1.70                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:57:G:H2'     | 1:AA:58:C:C6       | 2.23                     | 0.73              |
| 13:AM:15:VAL:HG12 | 13:AM:45:VAL:HG22  | 1.70                     | 0.73              |
| 27:BA:1686:C:H6   | 27:BA:1686:C:C5'   | 2.01                     | 0.73              |
| 27:BA:2728:U:C2'  | 27:BA:2729:G:H5'   | 2.18                     | 0.73              |
| 27:BA:633:A:H2'   | 27:BA:634:C:H5'    | 1.70                     | 0.73              |
| 27:BA:747:U:C5    | 54:B5:3:LYS:HB2    | 2.22                     | 0.73              |
| 30:BD:26:LYS:HZ3  | 30:BD:82:ILE:N     | 1.86                     | 0.73              |
| 39:BQ:118:LEU:CD1 | 39:BQ:131:ILE:HG23 | 2.17                     | 0.73              |
| 40:BR:23:ASN:HD22 | 40:BR:23:ASN:H     | 1.36                     | 0.73              |
| 44:BV:21:ARG:HB3  | 44:BV:91:TYR:HB2   | 1.70                     | 0.73              |
| 1:CA:350:G:H2'    | 1:CA:351:G:C8      | 2.23                     | 0.73              |
| 2:CB:69:LEU:HB3   | 2:CB:162:ILE:HG22  | 1.70                     | 0.73              |
| 2:CB:194:PRO:O    | 2:CB:196:LEU:HD12  | 1.87                     | 0.73              |
| 6:CF:3:ARG:HH11   | 6:CF:3:ARG:HG3     | 1.53                     | 0.73              |
| 39:DQ:81:VAL:CG2  | 49:D0:7:LEU:HD21   | 2.17                     | 0.73              |
| 51:D2:43:GLN:O    | 51:D2:44:LEU:HB2   | 1.87                     | 0.73              |
| 27:DA:2327:A:H2'  | 27:DA:2328:A:C8    | 2.24                     | 0.73              |
| 27:DA:2758:A:H2'  | 27:DA:2759:G:C5'   | 2.17                     | 0.73              |
| 38:DP:23:PRO:HD2  | 38:DP:33:ARG:NH2   | 2.02                     | 0.73              |
| 39:DQ:55:VAL:HG13 | 39:DQ:56:ARG:N     | 2.03                     | 0.73              |
| 39:DQ:79:LEU:HD22 | 39:DQ:80:GLU:HG3   | 1.68                     | 0.73              |
| 8:AH:27:PRO:O     | 8:AH:32:LYS:NZ     | 2.19                     | 0.73              |
| 20:AT:89:ARG:HD2  | 20:AT:104:LEU:HD11 | 1.69                     | 0.73              |
| 27:BA:1550:C:H2'  | 27:BA:1551:C:C6    | 2.23                     | 0.73              |
| 30:BD:44:ASN:HB3  | 30:BD:48:ARG:O     | 1.87                     | 0.73              |
| 31:BE:77:ILE:HG22 | 31:BE:78:LEU:N     | 1.98                     | 0.73              |
| 33:BG:103:LEU:HA  | 33:BG:106:LEU:HB3  | 1.70                     | 0.73              |
| 1:CA:1075:C:OP1   | 2:CB:103:THR:HG21  | 1.87                     | 0.73              |
| 1:CA:199:G:O2'    | 1:CA:200:G:H8      | 1.71                     | 0.73              |
| 3:CC:134:ILE:HD11 | 3:CC:153:VAL:HG23  | 1.70                     | 0.73              |
| 6:CF:33:TYR:HB2   | 6:CF:75:LEU:HD12   | 1.71                     | 0.73              |
| 7:CG:120:ILE:HG22 | 7:CG:124:LEU:HD12  | 1.70                     | 0.73              |
| 7:CG:59:LEU:O     | 7:CG:59:LEU:HD23   | 1.87                     | 0.73              |
| 1:CA:472:A:H4'    | 16:CP:82:GLN:HE22  | 1.52                     | 0.73              |
| 27:DA:1130:U:OP2  | 27:DA:2570:G:N2    | 2.18                     | 0.73              |
| 27:DA:1211:U:H4'  | 27:DA:1212:G:OP2   | 1.87                     | 0.73              |
| 27:DA:2572:A:H5'' | 27:DA:2574:G:C4'   | 2.17                     | 0.73              |
| 27:DA:484:C:H2'   | 27:DA:485:C:C6     | 2.22                     | 0.73              |
| 30:DD:35:LYS:O    | 30:DD:64:ILE:HG22  | 1.88                     | 0.73              |
| 31:DE:103:ASP:OD2 | 31:DE:201:THR:HA   | 1.87                     | 0.73              |
| 12:AL:10:LYS:HD2  | 12:AL:10:LYS:N     | 2.03                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:B2:41:ILE:HD11 | 51:B2:44:LEU:HB2   | 1.70                     | 0.73              |
| 13:AM:57:ARG:NH1  | 53:B4:60:GLU:HA    | 2.03                     | 0.73              |
| 34:BH:44:VAL:CG1  | 34:BH:45:VAL:H     | 1.99                     | 0.73              |
| 27:BA:483:A:HO2'  | 47:BY:60:PHE:HZ    | 1.34                     | 0.73              |
| 1:CA:116:A:H2'    | 1:CA:117:G:C8      | 2.21                     | 0.73              |
| 1:CA:1175:G:H2'   | 1:CA:1176:A:C8     | 2.24                     | 0.73              |
| 2:CB:147:LYS:HE2  | 2:CB:148:TYR:CE1   | 2.22                     | 0.73              |
| 19:CS:50:ALA:HB1  | 19:CS:57:HIS:HB3   | 1.70                     | 0.73              |
| 19:CS:60:VAL:HG21 | 19:CS:74:PHE:HB3   | 1.68                     | 0.73              |
| 57:D8:53:PRO:O    | 57:D8:56:GLU:N     | 2.19                     | 0.73              |
| 27:DA:1459:G:H2'  | 27:DA:1461:G:OP2   | 1.89                     | 0.73              |
| 37:DO:101:PRO:HD2 | 42:DT:70:VAL:CG2   | 2.18                     | 0.73              |
| 47:DY:43:ASN:HD21 | 47:DY:64:GLU:HG3   | 1.53                     | 0.73              |
| 4:AD:149:ALA:HB3  | 4:AD:152:SER:CB    | 2.18                     | 0.73              |
| 10:AJ:51:ARG:HG2  | 14:AN:45:ARG:NH1   | 2.03                     | 0.73              |
| 16:AP:2:VAL:HG23  | 16:AP:22:THR:O     | 1.89                     | 0.73              |
| 25:AY:65:U:H2'    | 25:AY:66:A:C8      | 2.23                     | 0.73              |
| 52:B3:8:LEU:HB2   | 52:B3:28:LEU:HD13  | 1.69                     | 0.73              |
| 1:CA:1296:C:H5'   | 13:CM:44:ARG:HH22  | 1.52                     | 0.73              |
| 1:CA:1524:C:H2'   | 1:CA:1525:G:C8     | 2.24                     | 0.73              |
| 1:CA:965:A:H4'    | 1:CA:966:G:OP1     | 1.88                     | 0.73              |
| 11:CK:123:LYS:HA  | 11:CK:126:ARG:HG3  | 1.70                     | 0.73              |
| 51:D2:16:LEU:H    | 51:D2:67:LYS:NZ    | 1.87                     | 0.73              |
| 27:DA:1496:A:H2'  | 27:DA:1498:C:C4    | 2.23                     | 0.73              |
| 27:DA:398:G:H2'   | 27:DA:399:G:H8     | 1.54                     | 0.73              |
| 27:DA:620:G:H4'   | 27:DA:621:A:H5''   | 1.71                     | 0.73              |
| 30:DD:153:ALA:C   | 30:DD:154:LYS:HG2  | 2.09                     | 0.73              |
| 38:DP:7:ARG:O     | 38:DP:10:PRO:CD    | 2.36                     | 0.73              |
| 48:DZ:39:ASP:HB3  | 48:DZ:42:GLU:HB2   | 1.70                     | 0.73              |
| 1:AA:1492:A:H2'   | 1:AA:1493:A:C8     | 2.24                     | 0.73              |
| 1:AA:918:A:H2'    | 1:AA:919:A:C8      | 2.24                     | 0.73              |
| 4:AD:98:GLU:HG3   | 4:AD:103:ASN:HD21  | 1.52                     | 0.73              |
| 27:BA:1417:C:H42  | 27:BA:1581:G:H1    | 1.35                     | 0.73              |
| 27:BA:2773:C:H2'  | 27:BA:2774:C:H6    | 1.54                     | 0.73              |
| 27:BA:29:U:H2'    | 27:BA:30:G:H8      | 1.54                     | 0.73              |
| 27:BA:940:G:H2'   | 27:BA:941:A:O4'    | 1.87                     | 0.73              |
| 28:BB:83:G:H1     | 28:BB:94:C:H42     | 1.34                     | 0.73              |
| 31:BE:68:ALA:C    | 31:BE:70:ALA:H     | 1.91                     | 0.73              |
| 33:BG:34:LEU:HA   | 33:BG:161:THR:HG23 | 1.71                     | 0.73              |
| 33:BG:47:LYS:HE2  | 33:BG:81:LYS:HE3   | 1.70                     | 0.73              |
| 35:BI:77:LEU:CD2  | 35:BI:78:THR:H     | 2.01                     | 0.73              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:BN:15:LEU:CD1    | 36:BN:136:GLU:HG2  | 2.19                     | 0.73              |
| 40:BR:10:LEU:HB3    | 40:BR:17:ARG:NE    | 2.03                     | 0.73              |
| 41:BS:16:ASN:ND2    | 41:BS:92:TYR:CE1   | 2.56                     | 0.73              |
| 1:CA:1086:U:H2'     | 1:CA:1087:G:O4'    | 1.88                     | 0.73              |
| 1:CA:1250:A:C5'     | 9:CI:67:GLY:HA2    | 2.17                     | 0.73              |
| 1:CA:1457:G:O2'     | 1:CA:1458:G:H5'    | 1.89                     | 0.73              |
| 12:CL:38:ARG:NH1    | 12:CL:38:ARG:HB3   | 2.03                     | 0.73              |
| 1:CA:1494:G:H8      | 26:CZ:3:SER:HB3    | 1.54                     | 0.73              |
| 27:DA:1305:C:O2'    | 27:DA:1306:C:H5'   | 1.88                     | 0.73              |
| 27:DA:1427:A:H4'    | 27:DA:1428:C:O5'   | 1.88                     | 0.73              |
| 27:DA:2258:C:H4'    | 27:DA:2259:G:OP2   | 1.88                     | 0.73              |
| 27:DA:2394:C:C2'    | 27:DA:2395:C:H5'   | 2.18                     | 0.73              |
| 27:DA:2493:U:C5     | 27:DA:2494:G:C8    | 2.76                     | 0.73              |
| 27:DA:2560:C:N4     | 27:DA:2561:A:N6    | 2.37                     | 0.73              |
| 27:DA:898:C:H2'     | 27:DA:899:A:H5'    | 1.71                     | 0.73              |
| 31:DE:154:LYS:O     | 31:DE:156:MET:HG3  | 1.88                     | 0.73              |
| 32:DF:184:TYR:CE2   | 32:DF:188:ARG:HD2  | 2.24                     | 0.73              |
| 34:DH:103:LEU:HD22  | 34:DH:123:PHE:CD2  | 2.23                     | 0.73              |
| 37:DO:97:ARG:O      | 37:DO:98:VAL:HG12  | 1.89                     | 0.73              |
| 1:AA:1187:G:OP1     | 9:AI:113:LYS:HE2   | 1.89                     | 0.73              |
| 1:AA:1424:C:H2'     | 1:AA:1425:U:O4'    | 1.89                     | 0.73              |
| 8:AH:54:ASP:HB2     | 8:AH:56:LYS:HE2    | 1.70                     | 0.73              |
| 20:AT:50:GLU:HG3    | 20:AT:51:GLU:H     | 1.54                     | 0.73              |
| 27:BA:1509(A):A:H2' | 27:BA:1509(B):A:C8 | 2.23                     | 0.73              |
| 36:BN:17:ASP:HB2    | 36:BN:55:VAL:CG1   | 2.19                     | 0.73              |
| 38:BP:50:ARG:HG2    | 38:BP:50:ARG:HH21  | 1.53                     | 0.73              |
| 41:BS:46:VAL:CG1    | 41:BS:47:THR:H     | 1.99                     | 0.73              |
| 47:BY:10:GLY:C      | 47:BY:27:VAL:HG22  | 2.09                     | 0.73              |
| 4:CD:200:GLU:HG2    | 4:CD:201:GLN:H     | 1.51                     | 0.73              |
| 11:CK:59:TYR:O      | 11:CK:62:GLN:HB3   | 1.88                     | 0.73              |
| 27:DA:2383:G:H2'    | 27:DA:2384:G:H8    | 1.52                     | 0.73              |
| 30:DD:77:ALA:HB2    | 30:DD:97:TYR:CE2   | 2.24                     | 0.73              |
| 31:DE:91:VAL:O      | 31:DE:92:THR:HG23  | 1.88                     | 0.73              |
| 35:DI:5:LEU:HD13    | 35:DI:17:GLN:HB3   | 1.70                     | 0.73              |
| 1:AA:1139:G:H4'     | 1:AA:1140:C:O5'    | 1.89                     | 0.73              |
| 1:AA:1391:U:H2'     | 1:AA:1392:G:C8     | 2.23                     | 0.73              |
| 2:AB:163:PHE:HA     | 2:AB:185:ILE:O     | 1.89                     | 0.73              |
| 9:AI:26:VAL:HG13    | 9:AI:61:ALA:HB3    | 1.70                     | 0.73              |
| 13:AM:24:GLY:C      | 13:AM:25:ILE:HD12  | 2.09                     | 0.73              |
| 16:AP:26:ARG:HD2    | 16:AP:31:LYS:O     | 1.88                     | 0.73              |
| 17:AQ:29:HIS:HE1    | 17:AQ:31:LEU:HB3   | 1.54                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:AQ:51:TYR:CE1   | 17:AQ:73:VAL:HG11  | 2.24                     | 0.73              |
| 51:B2:43:GLN:O     | 51:B2:44:LEU:HD22  | 1.89                     | 0.73              |
| 27:BA:271(S):G:C2' | 27:BA:271(T):C:H5' | 2.18                     | 0.73              |
| 30:BD:31:LYS:HD2   | 30:BD:33:LEU:HD13  | 1.70                     | 0.73              |
| 33:BG:2:PRO:C      | 33:BG:4:ASP:H      | 1.92                     | 0.73              |
| 1:CA:1342:C:H2'    | 1:CA:1343:G:H8     | 1.52                     | 0.73              |
| 1:CA:254:G:O2'     | 1:CA:255:G:H5'     | 1.87                     | 0.73              |
| 1:CA:397:A:H5''    | 1:CA:397:A:N3      | 2.03                     | 0.73              |
| 3:CC:83:ARG:O      | 3:CC:86:VAL:HG22   | 1.88                     | 0.73              |
| 4:CD:80:GLU:O      | 4:CD:84:LYS:HE2    | 1.89                     | 0.73              |
| 13:CM:93:ARG:C     | 13:CM:94:ARG:HD2   | 2.09                     | 0.73              |
| 24:CX:29:G:O2'     | 24:CX:30:G:H5'     | 1.89                     | 0.73              |
| 27:DA:2113:U:HO2'  | 27:DA:2114:A:H8    | 1.33                     | 0.73              |
| 27:DA:64:A:C5      | 46:DX:66:LEU:HD13  | 2.24                     | 0.73              |
| 32:DF:170:LEU:HD23 | 32:DF:173:VAL:HG23 | 1.71                     | 0.73              |
| 37:DO:8:LEU:HD22   | 37:DO:8:LEU:H      | 1.52                     | 0.73              |
| 46:DX:57:LEU:HD11  | 46:DX:78:LYS:HG2   | 1.71                     | 0.73              |
| 1:AA:967:C:H2'     | 1:AA:968:A:C8      | 2.24                     | 0.73              |
| 27:BA:857:C:C5'    | 49:B0:77:ARG:HH22  | 1.99                     | 0.73              |
| 27:BA:476:G:H4'    | 27:BA:502:A:N1     | 2.04                     | 0.73              |
| 31:BE:59:VAL:HG21  | 31:BE:63:LEU:HG    | 1.69                     | 0.73              |
| 34:BH:43:VAL:HG12  | 34:BH:53:GLU:H     | 1.53                     | 0.73              |
| 35:BI:132:PRO:HD2  | 35:BI:133:HIS:CD2  | 2.23                     | 0.73              |
| 43:BU:42:ALA:O     | 43:BU:44:ASN:N     | 2.22                     | 0.73              |
| 1:CA:832:C:O2'     | 1:CA:833:U:H5'     | 1.88                     | 0.73              |
| 1:CA:918:A:H2'     | 1:CA:919:A:C8      | 2.23                     | 0.73              |
| 1:CA:940:C:H2'     | 1:CA:941:G:H8      | 1.54                     | 0.73              |
| 3:CC:9:GLY:HA2     | 3:CC:12:LEU:HD23   | 1.70                     | 0.73              |
| 10:CJ:40:LEU:CD2   | 10:CJ:69:ASN:HB3   | 2.18                     | 0.73              |
| 14:CN:27:CYS:C     | 14:CN:29:ARG:H     | 1.91                     | 0.73              |
| 27:DA:1639:U:C2'   | 27:DA:1640:C:H5''  | 2.19                     | 0.73              |
| 27:DA:2192:G:H2'   | 27:DA:2193:G:H5''  | 1.71                     | 0.73              |
| 31:DE:188:VAL:CG2  | 31:DE:189:PRO:HD2  | 2.18                     | 0.73              |
| 34:DH:85:LYS:HZ2   | 34:DH:133:VAL:HG11 | 1.53                     | 0.73              |
| 1:AA:153:C:H2'     | 1:AA:154:C:C6      | 2.24                     | 0.73              |
| 12:AL:31:ARG:HG2   | 12:AL:32:GLY:H     | 1.52                     | 0.73              |
| 15:AO:55:GLY:HA2   | 15:AO:58:MET:CE    | 2.19                     | 0.73              |
| 20:AT:87:LYS:HG3   | 20:AT:91:LEU:HD11  | 1.71                     | 0.73              |
| 27:BA:1596:A:H2'   | 27:BA:1597:A:H5'   | 1.70                     | 0.73              |
| 27:BA:2306:C:C5    | 27:BA:2307:G:H1'   | 2.24                     | 0.73              |
| 27:BA:574:C:N4     | 31:BE:145:LYS:HE2  | 2.04                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:576:U:H2'    | 27:BA:577:G:C8     | 2.24                     | 0.73              |
| 27:BA:638:G:H2'    | 27:BA:639:U:O4'    | 1.89                     | 0.73              |
| 30:BD:117:VAL:HG22 | 30:BD:129:ASN:OD1  | 1.88                     | 0.73              |
| 30:BD:182:LEU:H    | 30:BD:272:ALA:HB3  | 1.54                     | 0.73              |
| 31:BE:9:VAL:HG11   | 31:BE:25:VAL:HG12  | 1.69                     | 0.73              |
| 35:BI:102:SER:HA   | 35:BI:107:VAL:H    | 1.52                     | 0.73              |
| 42:BT:28:VAL:CG2   | 42:BT:46:GLU:HA    | 2.17                     | 0.73              |
| 1:CA:1355:G:H2'    | 1:CA:1356:G:C8     | 2.24                     | 0.73              |
| 1:CA:16:A:N1       | 1:CA:919:A:H2      | 1.86                     | 0.73              |
| 4:CD:146:ILE:HD12  | 4:CD:146:ILE:H     | 1.54                     | 0.73              |
| 23:CW:30:A:H2'     | 23:CW:31:U:H5''    | 1.69                     | 0.73              |
| 27:DA:2067:G:O2'   | 27:DA:2068:U:OP1   | 2.05                     | 0.73              |
| 27:DA:2199:A:H5''  | 27:DA:2200:C:C5    | 2.22                     | 0.73              |
| 27:DA:917:A:H2'    | 27:DA:918:A:C8     | 2.23                     | 0.73              |
| 30:DD:174:ILE:O    | 30:DD:175:LEU:HD23 | 1.89                     | 0.73              |
| 1:AA:1287:A:H2'    | 1:AA:1288:A:C8     | 2.23                     | 0.72              |
| 1:AA:14:U:H2'      | 1:AA:16:A:OP2      | 1.88                     | 0.72              |
| 8:AH:116:LYS:HD3   | 8:AH:127:LEU:HD11  | 1.71                     | 0.72              |
| 9:AI:50:LEU:HA     | 9:AI:53:VAL:HG22   | 1.71                     | 0.72              |
| 13:AM:40:ASN:HD21  | 13:AM:42:ALA:HB3   | 1.53                     | 0.72              |
| 13:AM:96:LEU:HD22  | 13:AM:97:PRO:HD2   | 1.70                     | 0.72              |
| 16:AP:67:THR:O     | 16:AP:70:ALA:HB3   | 1.89                     | 0.72              |
| 18:AR:40:LEU:O     | 18:AR:43:PHE:N     | 2.23                     | 0.72              |
| 24:AX:2:G:H2'      | 24:AX:3:C:C6       | 2.23                     | 0.72              |
| 27:BA:1286:A:H2'   | 27:BA:1288:U:OP2   | 1.89                     | 0.72              |
| 27:BA:1750:G:O2'   | 27:BA:1751:C:H5'   | 1.89                     | 0.72              |
| 27:BA:200:U:H2'    | 27:BA:201:C:H5'    | 1.68                     | 0.72              |
| 30:BD:186:HIS:HD2  | 30:BD:188:GLU:H    | 0.85                     | 0.72              |
| 32:BF:16:GLY:O     | 32:BF:17:ARG:HG3   | 1.89                     | 0.72              |
| 33:BG:38:VAL:HG13  | 33:BG:92:VAL:O     | 1.88                     | 0.72              |
| 37:BO:71:ARG:NH1   | 42:BT:74:ARG:HH22  | 1.87                     | 0.72              |
| 47:BY:81:LYS:HD3   | 47:BY:97:ARG:HB3   | 1.71                     | 0.72              |
| 47:BY:81:LYS:NZ    | 47:BY:97:ARG:HG2   | 2.04                     | 0.72              |
| 1:CA:57:G:H2'      | 1:CA:58:C:C6       | 2.24                     | 0.72              |
| 1:CA:922:G:H2'     | 1:CA:923:A:H8      | 1.54                     | 0.72              |
| 2:CB:84:GLU:HB3    | 2:CB:219:VAL:HG21  | 1.71                     | 0.72              |
| 13:CM:37:THR:HG21  | 13:CM:56:LEU:HA    | 1.70                     | 0.72              |
| 13:CM:69:GLU:OE1   | 13:CM:72:ALA:HB3   | 1.88                     | 0.72              |
| 23:CW:42:G:C3'     | 23:CW:43:C:H5''    | 2.19                     | 0.72              |
| 49:D0:26:TYR:H     | 49:D0:29:GLN:NE2   | 1.77                     | 0.72              |
| 27:DA:143:G:H4'    | 46:DX:35:THR:HG21  | 1.70                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:1468:C:H2'  | 27:DA:1469:A:C8   | 2.23                     | 0.72              |
| 27:DA:1707:G:H2'  | 27:DA:1708:C:C6   | 2.24                     | 0.72              |
| 27:DA:1798:U:H5'  | 30:DD:259:THR:CG2 | 2.18                     | 0.72              |
| 27:DA:2758:A:C2'  | 27:DA:2759:G:H5'' | 2.19                     | 0.72              |
| 27:DA:476:G:N2    | 27:DA:478:A:H3'   | 2.04                     | 0.72              |
| 27:DA:543:C:N4    | 27:DA:551:G:H1    | 1.85                     | 0.72              |
| 35:DI:72:LEU:HD13 | 35:DI:75:LEU:HB3  | 1.71                     | 0.72              |
| 35:DI:83:ALA:HA   | 35:DI:89:TYR:CD1  | 2.23                     | 0.72              |
| 35:DI:83:ALA:HB2  | 35:DI:88:ILE:HA   | 1.71                     | 0.72              |
| 36:DN:125:GLY:HA3 | 36:DN:126:PRO:O   | 1.89                     | 0.72              |
| 1:AA:547:A:H4'    | 1:AA:548:G:O5'    | 1.89                     | 0.72              |
| 2:AB:164:VAL:O    | 2:AB:186:ALA:HB1  | 1.90                     | 0.72              |
| 9:AI:53:VAL:HG23  | 9:AI:55:ALA:N     | 2.03                     | 0.72              |
| 15:AO:61:GLY:O    | 15:AO:65:ARG:HD3  | 1.89                     | 0.72              |
| 18:AR:32:ARG:O    | 18:AR:69:THR:HG21 | 1.88                     | 0.72              |
| 52:B3:8:LEU:HD13  | 52:B3:31:LEU:HD23 | 1.71                     | 0.72              |
| 55:B6:39:TYR:O    | 55:B6:46:HIS:HB2  | 1.88                     | 0.72              |
| 27:BA:1108:U:H2'  | 27:BA:1109:C:H5'  | 1.69                     | 0.72              |
| 27:BA:2848:G:O2'  | 27:BA:2867:G:N2   | 2.22                     | 0.72              |
| 27:BA:610:G:H2'   | 27:BA:611:C:H6    | 1.54                     | 0.72              |
| 38:BP:18:ARG:O    | 38:BP:18:ARG:NH1  | 2.22                     | 0.72              |
| 38:BP:61:ARG:N    | 38:BP:61:ARG:HD2  | 2.03                     | 0.72              |
| 38:BP:84:ASN:HA   | 38:BP:115:LEU:O   | 1.89                     | 0.72              |
| 1:CA:365:U:H5'    | 1:CA:366:C:OP1    | 1.89                     | 0.72              |
| 8:CH:109:ILE:CG2  | 8:CH:137:VAL:HB   | 2.19                     | 0.72              |
| 17:CQ:44:ALA:HA   | 17:CQ:71:PHE:O    | 1.89                     | 0.72              |
| 1:CA:530:G:O6     | 22:CV:9:G:H1'     | 1.89                     | 0.72              |
| 56:D7:24:THR:HG23 | 56:D7:27:GLY:H    | 1.54                     | 0.72              |
| 27:DA:1385:G:H4'  | 27:DA:1386:C:OP1  | 1.88                     | 0.72              |
| 27:DA:1665:A:H4'  | 37:DO:67:LYS:HB2  | 1.71                     | 0.72              |
| 39:DQ:38:GLU:HG3  | 39:DQ:127:ILE:CG2 | 2.19                     | 0.72              |
| 27:DA:911:A:H2'   | 39:DQ:9:TYR:OH    | 1.90                     | 0.72              |
| 42:DT:27:THR:O    | 42:DT:28:VAL:HG23 | 1.89                     | 0.72              |
| 44:DV:12:TYR:CZ   | 44:DV:22:VAL:HG12 | 2.24                     | 0.72              |
| 47:DY:27:VAL:CA   | 47:DY:28:LYS:HZ1  | 2.00                     | 0.72              |
| 1:AA:1095:U:H5''  | 1:AA:1109:C:O2    | 1.89                     | 0.72              |
| 1:AA:598:U:H2'    | 1:AA:599:C:C6     | 2.24                     | 0.72              |
| 4:AD:2:GLY:O      | 4:AD:3:ARG:HD3    | 1.89                     | 0.72              |
| 12:AL:66:TYR:O    | 12:AL:68:PRO:HD3  | 1.89                     | 0.72              |
| 13:AM:74:VAL:HA   | 13:AM:77:ASN:HB3  | 1.69                     | 0.72              |
| 27:BA:2261:C:OP1  | 49:B0:17:GLN:NE2  | 2.20                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1150:C:O2'   | 27:BA:1151:G:H5'   | 1.90                     | 0.72              |
| 27:BA:1494:A:N3    | 27:BA:1494:A:H2'   | 2.04                     | 0.72              |
| 27:BA:1860:G:H1    | 27:BA:1882:C:N4    | 1.87                     | 0.72              |
| 27:BA:469:G:O6     | 56:B7:39:ARG:CZ    | 2.37                     | 0.72              |
| 30:BD:226:MET:O    | 30:BD:234:GLY:HA2  | 1.90                     | 0.72              |
| 30:BD:25:THR:C     | 30:BD:26:LYS:HD3   | 2.09                     | 0.72              |
| 30:BD:35:LYS:NZ    | 30:BD:103:ARG:CA   | 2.52                     | 0.72              |
| 31:BE:100:GLU:O    | 31:BE:172:VAL:HG23 | 1.90                     | 0.72              |
| 34:BH:10:PRO:CG    | 34:BH:50:VAL:H     | 2.01                     | 0.72              |
| 37:BO:78:ARG:HG3   | 37:BO:79:PHE:N     | 2.03                     | 0.72              |
| 1:CA:1129:C:H41    | 1:CA:1135:U:H3     | 1.35                     | 0.72              |
| 1:CA:1237:C:OP1    | 1:CA:1238:A:H1'    | 1.89                     | 0.72              |
| 1:CA:279:A:H5''    | 1:CA:281:G:O4'     | 1.89                     | 0.72              |
| 1:CA:743:U:H2'     | 1:CA:744:C:H6      | 1.54                     | 0.72              |
| 20:CT:89:ARG:NH2   | 20:CT:104:LEU:HD21 | 2.04                     | 0.72              |
| 25:CY:18:G:N2      | 25:CY:55:C:H42     | 1.87                     | 0.72              |
| 51:D2:50:ILE:C     | 51:D2:52:ASP:H     | 1.93                     | 0.72              |
| 27:DA:1925:C:C2'   | 27:DA:1926:U:H5'   | 2.19                     | 0.72              |
| 27:DA:352:G:O2'    | 27:DA:353:G:H3'    | 1.88                     | 0.72              |
| 28:DB:7:G:C3'      | 28:DB:8:U:H5''     | 2.18                     | 0.72              |
| 30:DD:85:ASP:HB2   | 30:DD:92:ILE:HD12  | 1.70                     | 0.72              |
| 32:DF:124:LEU:HB3  | 32:DF:193:VAL:HG22 | 1.70                     | 0.72              |
| 34:DH:13:LYS:CE    | 34:DH:13:LYS:HA    | 2.20                     | 0.72              |
| 42:DT:3:ARG:C      | 42:DT:5:ALA:H      | 1.91                     | 0.72              |
| 46:DX:92:LEU:O     | 46:DX:94:GLY:N     | 2.18                     | 0.72              |
| 1:AA:1528:U:O2'    | 1:AA:1529:G:H3'    | 1.89                     | 0.72              |
| 10:AJ:95:GLU:CD    | 10:AJ:96:ILE:H     | 1.93                     | 0.72              |
| 1:AA:1330:U:H4'    | 13:AM:23:TYR:CE2   | 2.23                     | 0.72              |
| 10:AJ:63:PHE:HA    | 14:AN:59:ALA:CB    | 2.20                     | 0.72              |
| 16:AP:18:ARG:NH1   | 16:AP:35:LYS:HD2   | 2.02                     | 0.72              |
| 27:BA:1482:G:N2    | 27:BA:1507:A:H1'   | 2.03                     | 0.72              |
| 27:BA:2162:G:H4'   | 27:BA:2172:U:O2'   | 1.88                     | 0.72              |
| 27:BA:2543:G:H8    | 27:BA:2543:G:H5'   | 1.52                     | 0.72              |
| 27:BA:271(I):G:H3' | 27:BA:271(J):C:H6  | 1.54                     | 0.72              |
| 31:BE:128:SER:O    | 31:BE:130:GLY:N    | 2.22                     | 0.72              |
| 34:BH:159:GLU:OE1  | 34:BH:159:GLU:HA   | 1.89                     | 0.72              |
| 36:BN:55:VAL:HG22  | 36:BN:126:PRO:HA   | 1.70                     | 0.72              |
| 27:BA:17:G:H4'     | 43:BU:25:TRP:CH2   | 2.24                     | 0.72              |
| 46:BX:9:LEU:HA     | 51:B2:36:ARG:NH2   | 2.05                     | 0.72              |
| 1:CA:718:G:H21     | 18:CR:49:LYS:HZ3   | 1.36                     | 0.72              |
| 5:CE:129:ILE:HD12  | 5:CE:129:ILE:H     | 1.52                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:CH:109:ILE:HG22 | 8:CH:137:VAL:HB    | 1.72                     | 0.72              |
| 8:CH:48:TYR:HD1   | 8:CH:49:GLU:N      | 1.87                     | 0.72              |
| 27:DA:2331:G:O2'  | 49:D0:43:THR:HG22  | 1.89                     | 0.72              |
| 27:DA:396:G:O4'   | 50:D1:13:ILE:HD11  | 1.89                     | 0.72              |
| 52:D3:7:LYS:HG2   | 52:D3:8:LEU:N      | 2.04                     | 0.72              |
| 27:DA:2282:G:O2'  | 27:DA:2283:C:OP2   | 2.07                     | 0.72              |
| 27:DA:66:C:H2'    | 27:DA:67:U:H6      | 1.55                     | 0.72              |
| 34:DH:92:ILE:HG22 | 34:DH:93:GLY:H     | 1.53                     | 0.72              |
| 46:DX:63:LYS:HB3  | 46:DX:72:LYS:HG3   | 1.70                     | 0.72              |
| 6:AF:61:LEU:O     | 6:AF:62:TRP:HB2    | 1.89                     | 0.72              |
| 27:BA:1400:G:O2'  | 27:BA:1401:G:H5'   | 1.89                     | 0.72              |
| 31:BE:145:LYS:O   | 31:BE:148:GLY:HA3  | 1.89                     | 0.72              |
| 32:BF:199:TRP:O   | 32:BF:203:GLN:HG3  | 1.89                     | 0.72              |
| 35:BI:81:VAL:HG21 | 35:BI:142:VAL:HG13 | 1.71                     | 0.72              |
| 1:CA:119:A:H4'    | 1:CA:120:A:O5'     | 1.87                     | 0.72              |
| 1:CA:1278:U:H5''  | 1:CA:1279:A:O4'    | 1.89                     | 0.72              |
| 6:CF:79:LEU:HD12  | 6:CF:88:VAL:HG11   | 1.71                     | 0.72              |
| 8:CH:109:ILE:HD11 | 8:CH:120:THR:CG2   | 2.18                     | 0.72              |
| 18:CR:32:ARG:HA   | 18:CR:69:THR:HG21  | 1.71                     | 0.72              |
| 27:DA:1041:C:H2'  | 27:DA:1042:G:H8    | 1.54                     | 0.72              |
| 27:DA:1322:A:H2'  | 27:DA:1323:U:H6    | 1.54                     | 0.72              |
| 1:CA:1494:G:H4'   | 27:DA:1913:A:N7    | 2.05                     | 0.72              |
| 27:DA:2531:A:H61  | 27:DA:2662:A:N6    | 1.88                     | 0.72              |
| 31:DE:26:ILE:HG22 | 31:DE:27:LEU:N     | 2.02                     | 0.72              |
| 40:DR:97:VAL:HG22 | 40:DR:114:VAL:HG22 | 1.70                     | 0.72              |
| 46:DX:48:LYS:HD2  | 46:DX:48:LYS:N     | 2.03                     | 0.72              |
| 1:AA:490:G:H2'    | 1:AA:491:G:C8      | 2.20                     | 0.72              |
| 4:AD:173:TRP:CD2  | 4:AD:189:PRO:HB3   | 2.25                     | 0.72              |
| 4:AD:188:LEU:HD22 | 4:AD:189:PRO:HD2   | 1.71                     | 0.72              |
| 50:B1:7:ILE:N     | 50:B1:7:ILE:HD12   | 2.04                     | 0.72              |
| 27:BA:1924:C:O2'  | 27:BA:1925:C:H5'   | 1.89                     | 0.72              |
| 27:BA:2122:U:H2'  | 27:BA:2123:G:H8    | 1.55                     | 0.72              |
| 27:BA:2443:C:O2'  | 27:BA:2444:G:H5'   | 1.90                     | 0.72              |
| 27:BA:2791:C:H4'  | 27:BA:2792:G:O5'   | 1.89                     | 0.72              |
| 27:BA:64:A:H1'    | 46:BX:66:LEU:HB2   | 1.69                     | 0.72              |
| 28:BB:94:C:O2'    | 28:BB:95:C:H5'     | 1.90                     | 0.72              |
| 44:BV:35:LEU:HB3  | 44:BV:37:VAL:HG23  | 1.72                     | 0.72              |
| 44:BV:39:LEU:O    | 44:BV:40:LEU:HB2   | 1.90                     | 0.72              |
| 47:BY:50:ARG:HG3  | 47:BY:58:GLY:HA3   | 1.71                     | 0.72              |
| 1:CA:508:C:H4'    | 1:CA:509:A:OP1     | 1.88                     | 0.72              |
| 1:CA:637:G:H2'    | 1:CA:638:G:C8      | 2.25                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:CG:20:ASP:HB3   | 7:CG:23:VAL:HG23  | 1.70                     | 0.72              |
| 17:CQ:59:ILE:HG22 | 17:CQ:71:PHE:CD1  | 2.24                     | 0.72              |
| 27:DA:1311:G:H21  | 27:DA:1603:A:H62  | 1.38                     | 0.72              |
| 27:DA:2276:G:OP1  | 39:DQ:84:GLY:HA2  | 1.90                     | 0.72              |
| 27:DA:244:A:O2'   | 38:DP:73:GLY:HA3  | 1.88                     | 0.72              |
| 28:DB:15:A:H5'    | 28:DB:16:G:H8     | 1.54                     | 0.72              |
| 27:DA:2757:A:C2   | 34:DH:67:LEU:HD22 | 2.23                     | 0.72              |
| 27:DA:662:G:H5'   | 38:DP:18:ARG:HA   | 1.72                     | 0.72              |
| 43:DU:66:ASN:O    | 43:DU:70:ARG:HG3  | 1.89                     | 0.72              |
| 43:DU:92:ARG:NH1  | 43:DU:92:ARG:HG2  | 1.97                     | 0.72              |
| 47:DY:28:LYS:CB   | 47:DY:38:ILE:H    | 2.01                     | 0.72              |
| 4:AD:59:ARG:NH2   | 4:AD:66:ARG:HH22  | 1.88                     | 0.72              |
| 6:AF:33:TYR:HB2   | 6:AF:75:LEU:HD12  | 1.70                     | 0.72              |
| 12:AL:86:ARG:HA   | 12:AL:94:ARG:HA   | 1.72                     | 0.72              |
| 16:AP:6:LEU:HB3   | 16:AP:17:TYR:HB3  | 1.70                     | 0.72              |
| 56:B7:37:LYS:HD3  | 56:B7:39:ARG:NE   | 2.05                     | 0.72              |
| 56:B7:8:ASN:ND2   | 56:B7:8:ASN:C     | 2.43                     | 0.72              |
| 27:BA:1686:C:H5'  | 27:BA:1686:C:H6   | 1.52                     | 0.72              |
| 27:BA:239:U:O2'   | 27:BA:240:G:H5'   | 1.88                     | 0.72              |
| 27:BA:572:A:H2'   | 27:BA:573:G:O4'   | 1.90                     | 0.72              |
| 32:BF:3:GLU:HA    | 32:BF:24:LEU:HG   | 1.71                     | 0.72              |
| 42:BT:33:LYS:HE3  | 42:BT:74:ARG:HH21 | 1.54                     | 0.72              |
| 42:BT:92:GLY:C    | 42:BT:94:ALA:N    | 2.41                     | 0.72              |
| 1:CA:578:C:N4     | 1:CA:763:G:H1     | 1.87                     | 0.72              |
| 1:CA:546:G:P      | 4:CD:72:GLU:HB3   | 2.30                     | 0.72              |
| 27:DA:1042:G:H1'  | 27:DA:1114:G:N2   | 2.03                     | 0.72              |
| 27:DA:1490:A:H5'  | 27:DA:1491:G:OP2  | 1.88                     | 0.72              |
| 27:DA:631:A:P     | 57:D8:46:ARG:HH21 | 2.13                     | 0.72              |
| 33:DG:125:PHE:HB2 | 33:DG:166:ASP:OD2 | 1.90                     | 0.72              |
| 33:DG:28:VAL:O    | 33:DG:31:VAL:N    | 2.23                     | 0.72              |
| 39:DQ:1:MET:O     | 39:DQ:2:LEU:HB2   | 1.90                     | 0.72              |
| 44:DV:59:ALA:HB2  | 44:DV:96:ILE:HA   | 1.71                     | 0.72              |
| 45:DW:21:VAL:O    | 45:DW:21:VAL:HG12 | 1.90                     | 0.72              |
| 3:AC:114:PRO:HG3  | 3:AC:185:GLY:HA3  | 1.71                     | 0.72              |
| 3:AC:186:PHE:HE2  | 3:AC:188:LEU:HD22 | 1.53                     | 0.72              |
| 5:AE:78:HIS:CE1   | 5:AE:142:LEU:HD23 | 2.25                     | 0.72              |
| 7:AG:143:ARG:HD2  | 25:AY:40:C:O2'    | 1.90                     | 0.72              |
| 55:B6:20:ASN:HD22 | 55:B6:21:TYR:N    | 1.86                     | 0.72              |
| 27:BA:2755:C:H3'  | 58:B9:19:ARG:HH21 | 1.53                     | 0.72              |
| 27:BA:191:A:H2'   | 27:BA:192:C:H6    | 1.53                     | 0.72              |
| 27:BA:2396:G:OP1  | 50:B1:25:LYS:NZ   | 2.23                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:744:G:OP1   | 31:BE:132:HIS:HB3  | 1.89                     | 0.72              |
| 27:BA:848:G:C4    | 27:BA:933:A:H8     | 2.08                     | 0.72              |
| 31:BE:54:GLN:O    | 31:BE:75:VAL:HG22  | 1.90                     | 0.72              |
| 33:BG:124:SER:HB2 | 33:BG:131:TYR:CE1  | 2.24                     | 0.72              |
| 35:BI:68:LEU:HA   | 35:BI:71:ILE:CG1   | 2.19                     | 0.72              |
| 38:BP:58:THR:O    | 38:BP:61:ARG:NE    | 2.22                     | 0.72              |
| 41:BS:24:LEU:HB3  | 41:BS:85:VAL:CG1   | 2.18                     | 0.72              |
| 1:CA:1343:G:H2'   | 1:CA:1344:C:C6     | 2.25                     | 0.72              |
| 1:CA:348:G:H2'    | 1:CA:349:A:C8      | 2.25                     | 0.72              |
| 1:CA:750:G:C2     | 15:CO:23:GLY:HA3   | 2.25                     | 0.72              |
| 13:CM:15:VAL:O    | 13:CM:19:LEU:HD22  | 1.90                     | 0.72              |
| 16:CP:21:VAL:HG12 | 16:CP:34:GLU:O     | 1.90                     | 0.72              |
| 25:CY:32:U:H2'    | 25:CY:34:U:OP2     | 1.89                     | 0.72              |
| 27:DA:1262:A:N3   | 54:D5:10:LYS:HE3   | 2.05                     | 0.72              |
| 27:DA:1722:A:N1   | 27:DA:1740:G:H8    | 1.86                     | 0.72              |
| 27:DA:94(A):G:H2' | 27:DA:95:G:C5'     | 2.16                     | 0.72              |
| 30:DD:65:ILE:N    | 30:DD:65:ILE:HD13  | 2.04                     | 0.72              |
| 33:DG:28:VAL:C    | 33:DG:30:GLU:N     | 2.43                     | 0.72              |
| 37:DO:87:ILE:HG23 | 37:DO:92:GLU:O     | 1.90                     | 0.72              |
| 45:DW:23:LEU:O    | 45:DW:27:LYS:HD2   | 1.89                     | 0.72              |
| 1:AA:583:A:N6     | 1:AA:758:G:H1'     | 2.04                     | 0.72              |
| 1:AA:823:G:O2'    | 1:AA:824:C:H5'     | 1.90                     | 0.72              |
| 23:AW:16:C:H4'    | 23:AW:59:U:O2'     | 1.89                     | 0.72              |
| 27:BA:593:G:H1'   | 57:B8:4:MET:HE1    | 1.71                     | 0.72              |
| 27:BA:2632:A:N3   | 31:BE:61:ARG:NH1   | 2.37                     | 0.72              |
| 27:BA:27:G:N2     | 27:BA:512:G:C2'    | 2.50                     | 0.72              |
| 27:BA:959:A:H5''  | 27:BA:959:A:H8     | 1.54                     | 0.72              |
| 42:BT:10:VAL:O    | 42:BT:10:VAL:HG12  | 1.88                     | 0.72              |
| 1:CA:1030:C:C2'   | 1:CA:1030(A):G:H5' | 2.19                     | 0.72              |
| 1:CA:335:C:H2'    | 1:CA:336:C:C6      | 2.25                     | 0.72              |
| 1:CA:880:C:H2'    | 1:CA:881:G:H8      | 1.51                     | 0.72              |
| 1:CA:983:A:H2'    | 1:CA:983:A:N3      | 2.03                     | 0.72              |
| 3:CC:39:ILE:HG22  | 3:CC:43:LEU:CD1    | 2.20                     | 0.72              |
| 54:D5:4:HIS:CB    | 54:D5:5:PRO:HD3    | 2.19                     | 0.72              |
| 27:DA:2355:C:H4'  | 49:D0:24:LYS:HG3   | 1.72                     | 0.72              |
| 27:DA:2515:C:H2'  | 27:DA:2516:G:H8    | 1.55                     | 0.72              |
| 27:DA:549:G:H2'   | 27:DA:551:G:H5''   | 1.72                     | 0.72              |
| 38:DP:21:ARG:HD3  | 38:DP:29:LYS:HE3   | 1.71                     | 0.72              |
| 7:AG:15:ASP:O     | 7:AG:19:GLY:HA2    | 1.90                     | 0.72              |
| 52:B3:11:SER:HG   | 52:B3:13:ILE:HD12  | 1.55                     | 0.72              |
| 57:B8:37:SER:O    | 57:B8:40:GLU:HB2   | 1.90                     | 0.72              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 57:B8:51:ALA:C     | 57:B8:53:PRO:HD2  | 2.10                     | 0.72              |
| 27:BA:2320:A:H2'   | 27:BA:2320:A:N3   | 2.05                     | 0.72              |
| 31:BE:81:ILE:O     | 31:BE:81:ILE:HG22 | 1.90                     | 0.72              |
| 37:BO:2:ILE:N      | 37:BO:2:ILE:HD13  | 2.04                     | 0.72              |
| 37:BO:77:ILE:HD11  | 42:BT:72:VAL:CG1  | 2.20                     | 0.72              |
| 38:BP:48:PRO:HG2   | 38:BP:49:ARG:N    | 2.05                     | 0.72              |
| 40:BR:101:ALA:O    | 40:BR:102:GLU:HB2 | 1.89                     | 0.72              |
| 40:BR:45:ARG:O     | 40:BR:48:VAL:HG23 | 1.89                     | 0.72              |
| 40:BR:4:LEU:O      | 40:BR:4:LEU:HD13  | 1.88                     | 0.72              |
| 46:BX:12:VAL:HG12  | 46:BX:27:THR:OG1  | 1.89                     | 0.72              |
| 1:CA:1060:C:O2'    | 1:CA:1061:G:H5'   | 1.89                     | 0.72              |
| 1:CA:1116:C:H2'    | 1:CA:1117:G:H5''  | 1.70                     | 0.72              |
| 1:CA:93:G:H2'      | 1:CA:96:U:H5'     | 1.71                     | 0.72              |
| 1:CA:994:A:N7      | 1:CA:1216:G:H4'   | 2.05                     | 0.72              |
| 1:CA:36:C:H4'      | 12:CL:119:THR:O   | 1.90                     | 0.72              |
| 17:CQ:57:VAL:HG12  | 17:CQ:76:LEU:CA   | 2.18                     | 0.72              |
| 27:DA:2080:G:OP1   | 50:D1:35:THR:HG21 | 1.89                     | 0.72              |
| 58:D9:11:CYS:SG    | 58:D9:32:HIS:CE1  | 2.83                     | 0.72              |
| 27:DA:1449:A:H5'   | 27:DA:1450:G:OP2  | 1.89                     | 0.72              |
| 27:DA:1925:C:O2'   | 27:DA:1926:U:H5'  | 1.90                     | 0.72              |
| 27:DA:363(E):U:H5' | 27:DA:363(F):A:C8 | 2.25                     | 0.72              |
| 27:DA:930:U:H4'    | 27:DA:931:G:C4    | 2.25                     | 0.72              |
| 34:DH:23:ARG:O     | 34:DH:24:VAL:HG13 | 1.89                     | 0.72              |
| 35:DI:107:VAL:HG12 | 35:DI:108:THR:N   | 2.04                     | 0.72              |
| 38:DP:17:LYS:O     | 38:DP:17:LYS:HG2  | 1.88                     | 0.72              |
| 27:DA:587:C:C4     | 38:DP:33:ARG:HD3  | 2.25                     | 0.72              |
| 45:DW:83:LYS:HA    | 45:DW:97:LYS:HG2  | 1.71                     | 0.72              |
| 8:AH:48:TYR:HA     | 8:AH:60:ARG:O     | 1.89                     | 0.71              |
| 11:AK:86:GLY:N     | 11:AK:112:THR:OG1 | 2.22                     | 0.71              |
| 27:BA:2637:U:H2'   | 27:BA:2638:G:H5'  | 1.71                     | 0.71              |
| 27:BA:977:G:O2'    | 27:BA:978:G:H5'   | 1.90                     | 0.71              |
| 31:BE:57:LYS:C     | 31:BE:59:VAL:H    | 1.93                     | 0.71              |
| 35:BI:8:PRO:HB3    | 35:BI:14:ASP:HA   | 1.70                     | 0.71              |
| 38:BP:112:LEU:H    | 38:BP:128:HIS:CD2 | 2.04                     | 0.71              |
| 38:BP:84:ASN:HD22  | 38:BP:115:LEU:HG  | 1.53                     | 0.71              |
| 47:BY:96:ILE:CG2   | 47:BY:97:ARG:N    | 2.52                     | 0.71              |
| 1:CA:148:G:H1      | 1:CA:174:C:N4     | 1.88                     | 0.71              |
| 1:CA:377:G:H1      | 1:CA:386:C:N4     | 1.86                     | 0.71              |
| 12:CL:123:LYS:C    | 12:CL:125:ALA:H   | 1.93                     | 0.71              |
| 57:D8:50:LEU:HD12  | 57:D8:51:ALA:N    | 2.04                     | 0.71              |
| 27:DA:2080:G:P     | 50:D1:35:THR:HG21 | 2.30                     | 0.71              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:768:G:H2'    | 27:DA:769:G:C8    | 2.25                     | 0.71              |
| 38:DP:146:VAL:HG22 | 38:DP:147:LEU:N   | 2.05                     | 0.71              |
| 1:AA:1036:G:H5'    | 1:AA:1037:C:OP2   | 1.89                     | 0.71              |
| 1:AA:246:A:H4'     | 1:AA:247:G:OP1    | 1.89                     | 0.71              |
| 4:AD:25:ARG:HG2    | 4:AD:25:ARG:HH11  | 1.55                     | 0.71              |
| 15:AO:28:GLN:O     | 15:AO:32:LEU:HG   | 1.88                     | 0.71              |
| 19:AS:64:GLU:O     | 19:AS:67:VAL:HG22 | 1.90                     | 0.71              |
| 25:AY:71:A:H2'     | 25:AY:72:G:H8     | 1.52                     | 0.71              |
| 49:B0:65:GLY:HA3   | 49:B0:83:PRO:HA   | 1.71                     | 0.71              |
| 27:BA:1948:G:O2'   | 27:BA:1949:G:H5'  | 1.90                     | 0.71              |
| 27:BA:2428:G:H5''  | 27:BA:2429:G:O5'  | 1.89                     | 0.71              |
| 30:BD:168:ARG:O    | 30:BD:169:GLU:HB2 | 1.90                     | 0.71              |
| 32:BF:28:ILE:O     | 32:BF:28:ILE:HD12 | 1.90                     | 0.71              |
| 39:BQ:135:ASP:O    | 39:BQ:137:TYR:N   | 2.21                     | 0.71              |
| 45:BW:10:VAL:HG23  | 45:BW:101:SER:O   | 1.90                     | 0.71              |
| 1:CA:1068:G:N7     | 1:CA:1094:G:C8    | 2.58                     | 0.71              |
| 1:CA:1215:G:H2'    | 1:CA:1216:G:H8    | 1.55                     | 0.71              |
| 1:CA:59:A:H5'      | 1:CA:60:A:H5'     | 1.71                     | 0.71              |
| 1:CA:839:U:H2'     | 1:CA:839:U:O2     | 1.89                     | 0.71              |
| 1:CA:991:U:O2      | 1:CA:991:U:H2'    | 1.89                     | 0.71              |
| 11:CK:96:ARG:HA    | 11:CK:99:GLN:HG2  | 1.71                     | 0.71              |
| 12:CL:107:VAL:CG2  | 12:CL:117:TYR:HB3 | 2.20                     | 0.71              |
| 24:CX:17:C:H3'     | 24:CX:17(B):U:C5' | 2.20                     | 0.71              |
| 27:DA:1197:G:O2'   | 27:DA:1198:U:H5'  | 1.91                     | 0.71              |
| 27:DA:1654:A:P     | 40:DR:3:HIS:HB2   | 2.30                     | 0.71              |
| 27:DA:2757:A:N1    | 34:DH:67:LEU:HD13 | 2.05                     | 0.71              |
| 31:DE:2:LYS:HE2    | 31:DE:95:ILE:HG23 | 1.72                     | 0.71              |
| 27:DA:1242:A:N1    | 38:DP:8:PRO:HG3   | 2.04                     | 0.71              |
| 39:DQ:43:THR:HG22  | 39:DQ:94:VAL:HG12 | 1.72                     | 0.71              |
| 48:DZ:150:HIS:HB3  | 48:DZ:169:THR:CG2 | 2.16                     | 0.71              |
| 1:AA:542:G:H5'     | 4:AD:41:GLY:HA3   | 1.73                     | 0.71              |
| 3:AC:87:LEU:C      | 3:AC:89:GLU:N     | 2.43                     | 0.71              |
| 8:AH:127:LEU:HD12  | 8:AH:129:VAL:HG13 | 1.73                     | 0.71              |
| 10:AJ:48:THR:HA    | 10:AJ:62:HIS:HB3  | 1.71                     | 0.71              |
| 16:AP:6:LEU:HD12   | 16:AP:6:LEU:N     | 2.04                     | 0.71              |
| 25:AY:63:C:H2'     | 25:AY:64:G:C8     | 2.25                     | 0.71              |
| 27:BA:2023:G:H5'   | 27:BA:2617:C:H4'  | 1.72                     | 0.71              |
| 27:BA:2619:C:O2'   | 27:BA:2620:C:H5'  | 1.89                     | 0.71              |
| 27:BA:469:G:O2'    | 27:BA:470:A:H5''  | 1.90                     | 0.71              |
| 30:BD:26:LYS:NZ    | 30:BD:82:ILE:N    | 2.37                     | 0.71              |
| 33:BG:128:ARG:HB2  | 33:BG:130:ASN:O   | 1.91                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2685:G:H5'   | 37:BO:68:GLU:OE2   | 1.90                     | 0.71              |
| 1:CA:500:G:H2'     | 1:CA:501:C:C6      | 2.25                     | 0.71              |
| 1:CA:624:C:O2'     | 1:CA:625:G:H5'     | 1.90                     | 0.71              |
| 1:CA:792:A:H4'     | 1:CA:793:U:O5'     | 1.90                     | 0.71              |
| 3:CC:39:ILE:C      | 3:CC:41:GLY:H      | 1.94                     | 0.71              |
| 7:CG:49:ILE:CG2    | 7:CG:53:LYS:HD2    | 2.19                     | 0.71              |
| 13:CM:116:THR:O    | 13:CM:117:VAL:HB   | 1.90                     | 0.71              |
| 15:CO:56:LEU:O     | 15:CO:60:VAL:HG23  | 1.90                     | 0.71              |
| 27:DA:150:C:H2'    | 27:DA:151:C:C6     | 2.24                     | 0.71              |
| 27:DA:172:C:HO2'   | 27:DA:173:G:H8     | 1.38                     | 0.71              |
| 27:DA:740:U:H2'    | 27:DA:741:G:C8     | 2.25                     | 0.71              |
| 28:DB:88:C:H2'     | 28:DB:89:G:C8      | 2.24                     | 0.71              |
| 32:DF:132:VAL:HG13 | 32:DF:133:ASN:N    | 2.05                     | 0.71              |
| 48:DZ:107:PRO:C    | 48:DZ:109:GLY:H    | 1.92                     | 0.71              |
| 48:DZ:117:GLN:HG2  | 48:DZ:118:GLU:N    | 2.05                     | 0.71              |
| 1:AA:532:A:H3'     | 1:AA:533:A:C5'     | 2.20                     | 0.71              |
| 2:AB:197:VAL:HB    | 2:AB:200:ILE:HG12  | 1.71                     | 0.71              |
| 1:AA:1080:A:C5'    | 5:AE:14:ARG:HH21   | 1.92                     | 0.71              |
| 10:AJ:96:ILE:HD13  | 10:AJ:96:ILE:H     | 1.55                     | 0.71              |
| 19:AS:15:LEU:O     | 19:AS:19:VAL:HG23  | 1.90                     | 0.71              |
| 27:BA:271(Q):G:H2' | 27:BA:271(R):G:H8  | 1.55                     | 0.71              |
| 27:BA:2808:U:H5'   | 27:BA:2891:G:O6    | 1.88                     | 0.71              |
| 27:BA:29:U:H2'     | 27:BA:30:G:C8      | 2.25                     | 0.71              |
| 27:BA:40:C:H2'     | 27:BA:41:C:H6      | 1.54                     | 0.71              |
| 27:BA:747:U:C2     | 54:B5:2:ALA:N      | 2.58                     | 0.71              |
| 29:BC:75:LEU:HD21  | 29:BC:99:ILE:HD12  | 1.71                     | 0.71              |
| 34:BH:121:ILE:HD11 | 34:BH:140:LYS:O    | 1.91                     | 0.71              |
| 34:BH:46:GLU:HG3   | 34:BH:51:ARG:HB2   | 1.73                     | 0.71              |
| 42:BT:102:ILE:HB   | 42:BT:110:ILE:HD11 | 1.72                     | 0.71              |
| 1:CA:1412:C:H2'    | 1:CA:1413:A:C8     | 2.25                     | 0.71              |
| 4:CD:9:CYS:HB2     | 4:CD:22:LYS:NZ     | 2.06                     | 0.71              |
| 5:CE:80:ILE:HD13   | 5:CE:138:ALA:HB1   | 1.71                     | 0.71              |
| 12:CL:3:THR:HG22   | 12:CL:6:GLN:NE2    | 2.05                     | 0.71              |
| 14:CN:22:THR:OG1   | 14:CN:33:VAL:HG21  | 1.90                     | 0.71              |
| 1:CA:235:C:H1'     | 17:CQ:61:GLU:OE1   | 1.90                     | 0.71              |
| 23:CW:30:A:H2'     | 23:CW:31:U:C5'     | 2.21                     | 0.71              |
| 27:DA:224:G:H2'    | 27:DA:225:A:O4'    | 1.90                     | 0.71              |
| 27:DA:2303:G:H1'   | 33:DG:132:ASN:ND2  | 2.05                     | 0.71              |
| 27:DA:2350:C:H41   | 27:DA:2382:G:N2    | 1.88                     | 0.71              |
| 27:DA:2791:C:H4'   | 27:DA:2792:G:O5'   | 1.90                     | 0.71              |
| 27:DA:94:C:H5'     | 27:DA:94(A):G:OP2  | 1.91                     | 0.71              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DF:125:LEU:HB3  | 32:DF:196:LEU:CD2 | 2.21                     | 0.71              |
| 35:DI:88:ILE:HD11  | 35:DI:123:LEU:HG  | 1.72                     | 0.71              |
| 46:DX:57:LEU:CD1   | 46:DX:78:LYS:HG2  | 2.19                     | 0.71              |
| 47:DY:45:VAL:HG13  | 47:DY:62:GLU:OE2  | 1.91                     | 0.71              |
| 48:DZ:128:SER:OG   | 48:DZ:130:ARG:HD3 | 1.89                     | 0.71              |
| 1:AA:1286:A:H2'    | 1:AA:1287:A:H4'   | 1.72                     | 0.71              |
| 1:AA:736:C:H2'     | 1:AA:737:A:H8     | 1.55                     | 0.71              |
| 5:AE:100:VAL:HG23  | 5:AE:116:THR:O    | 1.91                     | 0.71              |
| 5:AE:99:GLY:O      | 5:AE:117:ASP:HA   | 1.90                     | 0.71              |
| 27:BA:1192:G:O2'   | 27:BA:1193:G:H5'' | 1.89                     | 0.71              |
| 27:BA:183:C:H1'    | 27:BA:433:C:H1'   | 1.71                     | 0.71              |
| 27:BA:1963:U:H2'   | 27:BA:1963:U:O2   | 1.90                     | 0.71              |
| 27:BA:347:A:H2'    | 27:BA:348:G:H8    | 1.54                     | 0.71              |
| 32:BF:175:THR:HG23 | 32:BF:175:THR:O   | 1.90                     | 0.71              |
| 35:BI:68:LEU:HD23  | 35:BI:68:LEU:O    | 1.90                     | 0.71              |
| 40:BR:67:LEU:HD22  | 40:BR:76:VAL:HG21 | 1.71                     | 0.71              |
| 43:BU:95:LEU:HD22  | 44:BV:4:ILE:CD1   | 2.21                     | 0.71              |
| 45:BW:64:MET:O     | 45:BW:65:LEU:HB2  | 1.90                     | 0.71              |
| 45:BW:85:VAL:HG12  | 45:BW:86:LEU:N    | 2.06                     | 0.71              |
| 1:CA:1036:G:H5'    | 1:CA:1037:C:OP2   | 1.90                     | 0.71              |
| 1:CA:1258:G:H2'    | 1:CA:1259:C:C6    | 2.26                     | 0.71              |
| 3:CC:116:VAL:O     | 3:CC:119:ARG:HB3  | 1.90                     | 0.71              |
| 3:CC:11:ARG:HH11   | 3:CC:11:ARG:HG2   | 1.55                     | 0.71              |
| 1:CA:921:U:O2      | 5:CE:19:MET:HB2   | 1.89                     | 0.71              |
| 13:CM:36:LYS:HZ3   | 13:CM:59:TYR:HE1  | 1.37                     | 0.71              |
| 27:DA:1515:G:C2'   | 27:DA:1516:C:H5'  | 2.21                     | 0.71              |
| 27:DA:2550:G:H2'   | 27:DA:2551:C:H5'  | 1.72                     | 0.71              |
| 27:DA:27:G:N2      | 27:DA:512:G:H2'   | 2.05                     | 0.71              |
| 27:DA:297:C:H2'    | 27:DA:298:G:O4'   | 1.90                     | 0.71              |
| 27:DA:288:C:N4     | 27:DA:353:G:H1    | 1.87                     | 0.71              |
| 27:DA:975(A):G:H21 | 27:DA:976:C:H1'   | 1.54                     | 0.71              |
| 31:DE:29:GLY:HA2   | 31:DE:180:ASN:HB3 | 1.72                     | 0.71              |
| 32:DF:143:ALA:O    | 32:DF:148:LEU:HB2 | 1.90                     | 0.71              |
| 35:DI:31:LEU:HB2   | 35:DI:32:PRO:HD3  | 1.73                     | 0.71              |
| 35:DI:71:ILE:HG13  | 35:DI:72:LEU:N    | 2.04                     | 0.71              |
| 38:DP:112:LEU:HD22 | 38:DP:113:LYS:N   | 2.04                     | 0.71              |
| 45:DW:44:ALA:O     | 45:DW:47:VAL:N    | 2.22                     | 0.71              |
| 1:AA:1064:G:N2     | 1:AA:1190:G:H2'   | 2.06                     | 0.71              |
| 10:AJ:49:VAL:CG2   | 14:AN:41:ARG:HD2  | 2.21                     | 0.71              |
| 27:BA:1051:G:O2'   | 27:BA:1052:C:H6   | 1.73                     | 0.71              |
| 27:BA:1570:A:H2'   | 27:BA:1571:A:C8   | 2.25                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1722:A:N1    | 27:BA:1740:G:H8    | 1.88                     | 0.71              |
| 27:BA:1956:U:H2'   | 27:BA:1957:C:H5'   | 1.71                     | 0.71              |
| 27:BA:2263:C:H2'   | 27:BA:2264:C:C6    | 2.20                     | 0.71              |
| 27:BA:2756:U:OP2   | 58:B9:19:ARG:NH2   | 2.21                     | 0.71              |
| 27:BA:2787:C:H1'   | 31:BE:61:ARG:CG    | 2.13                     | 0.71              |
| 27:BA:2808:U:O2'   | 27:BA:2809:A:H5'   | 1.89                     | 0.71              |
| 27:BA:2832:U:H4'   | 27:BA:2833:G:C5'   | 2.19                     | 0.71              |
| 27:BA:858:U:H4'    | 27:BA:859:G:OP1    | 1.90                     | 0.71              |
| 27:BA:863:A:H2'    | 27:BA:864:G:C8     | 2.25                     | 0.71              |
| 30:BD:158:ALA:HB3  | 30:BD:161:THR:CG2  | 2.21                     | 0.71              |
| 27:BA:1813:G:H4'   | 30:BD:44:ASN:O     | 1.90                     | 0.71              |
| 34:BH:86:GLU:CB    | 34:BH:132:ARG:HH12 | 2.03                     | 0.71              |
| 45:BW:90:ARG:HB2   | 45:BW:90:ARG:NH1   | 2.04                     | 0.71              |
| 1:CA:128:G:O2'     | 1:CA:129:U:H5'     | 1.89                     | 0.71              |
| 1:CA:372:C:H5'     | 1:CA:373:A:OP1     | 1.91                     | 0.71              |
| 1:CA:407:G:H2'     | 1:CA:408:A:H8      | 1.55                     | 0.71              |
| 11:CK:32:ILE:HD12  | 11:CK:72:ALA:CB    | 2.18                     | 0.71              |
| 6:CF:50:TYR:CE1    | 18:CR:77:GLY:HA2   | 2.24                     | 0.71              |
| 49:D0:49:LYS:HB2   | 49:D0:80:HIS:HB3   | 1.71                     | 0.71              |
| 51:D2:63:VAL:O     | 51:D2:66:GLU:HG2   | 1.91                     | 0.71              |
| 52:D3:23:LEU:N     | 52:D3:23:LEU:HD12  | 2.04                     | 0.71              |
| 27:DA:1292:U:H2'   | 27:DA:1293:C:O4'   | 1.90                     | 0.71              |
| 27:DA:1639:U:O2'   | 27:DA:1640:C:H5''  | 1.89                     | 0.71              |
| 27:DA:2468:G:H22   | 27:DA:2481:G:H2'   | 1.56                     | 0.71              |
| 27:DA:2512:C:H4'   | 31:DE:122:PHE:CE2  | 2.25                     | 0.71              |
| 27:DA:2884:U:H2'   | 27:DA:2885:C:H5'   | 1.71                     | 0.71              |
| 27:DA:482:A:H62    | 27:DA:506:G:H2'    | 1.56                     | 0.71              |
| 29:DC:122:ALA:HB1  | 29:DC:129:ARG:CB   | 2.21                     | 0.71              |
| 31:DE:110:GLY:HA2  | 31:DE:162:ALA:H    | 1.54                     | 0.71              |
| 33:DG:101:ILE:HD11 | 33:DG:105:LYS:NZ   | 2.05                     | 0.71              |
| 33:DG:128:ARG:C    | 33:DG:130:ASN:H    | 1.94                     | 0.71              |
| 33:DG:41:GLN:HE22  | 33:DG:153:ARG:HG2  | 1.55                     | 0.71              |
| 1:AA:1132:C:O2'    | 1:AA:1133:G:H5'    | 1.90                     | 0.71              |
| 1:AA:664:G:H22     | 1:AA:741:G:H1      | 1.39                     | 0.71              |
| 4:AD:100:ARG:NH1   | 4:AD:137:SER:HB3   | 2.06                     | 0.71              |
| 6:AF:75:LEU:HD23   | 6:AF:75:LEU:C      | 2.10                     | 0.71              |
| 8:AH:32:LYS:O      | 8:AH:35:ILE:HB     | 1.90                     | 0.71              |
| 9:AI:122:ALA:HB1   | 9:AI:123:PRO:HD2   | 1.72                     | 0.71              |
| 19:AS:32:LYS:CA    | 19:AS:50:ALA:HB3   | 2.20                     | 0.71              |
| 1:AA:262:A:H5'     | 20:AT:74:LYS:CG    | 2.20                     | 0.71              |
| 27:BA:686:G:N3     | 56:B7:11:LYS:HE3   | 2.05                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:B8:32:LEU:N     | 57:B8:33:ASN:HD22  | 1.89                     | 0.71              |
| 27:BA:2073:C:O2'   | 27:BA:2074:U:H5'   | 1.89                     | 0.71              |
| 27:BA:225:A:H2'    | 27:BA:226:G:H5'    | 1.71                     | 0.71              |
| 27:BA:2346:A:C8    | 27:BA:2383:G:C5    | 2.79                     | 0.71              |
| 27:BA:2667:C:H1'   | 34:BH:109:PHE:CD2  | 2.25                     | 0.71              |
| 27:BA:592:G:H1     | 27:BA:665:C:H42    | 1.36                     | 0.71              |
| 30:BD:60:ARG:CD    | 30:BD:86:PRO:HB2   | 2.20                     | 0.71              |
| 30:BD:60:ARG:NE    | 30:BD:86:PRO:HB2   | 2.05                     | 0.71              |
| 31:BE:104:VAL:HG11 | 31:BE:188:VAL:HG23 | 1.71                     | 0.71              |
| 42:BT:23:ARG:HG2   | 42:BT:120:ARG:HH12 | 1.56                     | 0.71              |
| 48:BZ:101:LEU:HD11 | 48:BZ:123:ILE:HG22 | 1.72                     | 0.71              |
| 1:CA:627:G:H2'     | 1:CA:628:G:C8      | 2.25                     | 0.71              |
| 1:CA:707:C:H2'     | 1:CA:708:C:C6      | 2.25                     | 0.71              |
| 1:CA:860:A:H2'     | 1:CA:861:G:O4'     | 1.90                     | 0.71              |
| 4:CD:173:TRP:HA    | 4:CD:187:ARG:NH1   | 2.05                     | 0.71              |
| 7:CG:72:ARG:O      | 7:CG:73:MET:HG3    | 1.90                     | 0.71              |
| 19:CS:9:VAL:O      | 19:CS:11:VAL:N     | 2.24                     | 0.71              |
| 55:D6:40:CYS:CB    | 55:D6:46:HIS:HB3   | 2.20                     | 0.71              |
| 27:DA:1205:U:H4'   | 27:DA:1206:G:OP2   | 1.91                     | 0.71              |
| 27:DA:1260:G:H2'   | 27:DA:1261:C:C6    | 2.26                     | 0.71              |
| 27:DA:1848:A:C2    | 27:DA:1849:G:H1'   | 2.26                     | 0.71              |
| 27:DA:2308:G:O6    | 27:DA:2310:A:H5'   | 1.89                     | 0.71              |
| 27:DA:2351:G:H2'   | 27:DA:2365:G:N2    | 2.05                     | 0.71              |
| 27:DA:2756:U:O2'   | 27:DA:2757:A:H5'   | 1.90                     | 0.71              |
| 27:DA:536:A:H2'    | 27:DA:537:C:C6     | 2.24                     | 0.71              |
| 28:DB:111:G:H2'    | 28:DB:112:U:O4'    | 1.89                     | 0.71              |
| 37:DO:24:VAL:HA    | 37:DO:39:ILE:HG22  | 1.72                     | 0.71              |
| 37:DO:2:ILE:HG21   | 37:DO:8:LEU:HD11   | 1.71                     | 0.71              |
| 38:DP:9:ASN:H      | 38:DP:10:PRO:CD    | 2.02                     | 0.71              |
| 46:DX:64:LYS:HZ3   | 46:DX:73:ARG:NH2   | 1.87                     | 0.71              |
| 47:DY:75:ILE:HB    | 47:DY:80:GLY:H     | 1.54                     | 0.71              |
| 47:DY:88:LYS:HD3   | 47:DY:93:GLY:H     | 1.56                     | 0.71              |
| 2:AB:178:ARG:NH2   | 8:AH:68:ARG:NH2    | 2.38                     | 0.71              |
| 14:AN:23:ARG:HD2   | 14:AN:28:GLY:O     | 1.90                     | 0.71              |
| 55:B6:40:CYS:HA    | 55:B6:46:HIS:HB2   | 1.70                     | 0.71              |
| 55:B6:26:ASN:ND2   | 55:B6:51:GLU:OE1   | 2.24                     | 0.71              |
| 27:BA:2178:C:H4'   | 29:BC:46:LYS:HD3   | 1.72                     | 0.71              |
| 34:BH:43:VAL:CG1   | 34:BH:52:VAL:HA    | 2.21                     | 0.71              |
| 27:BA:662:G:OP1    | 38:BP:18:ARG:HD2   | 1.89                     | 0.71              |
| 45:BW:5:ALA:C      | 45:BW:6:ILE:HG13   | 2.11                     | 0.71              |
| 39:BQ:108:GLY:HA3  | 48:BZ:115:VAL:HG11 | 1.71                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:254:G:OP1     | 17:CQ:67:LYS:O     | 2.08                     | 0.71              |
| 1:CA:59:A:C5'      | 1:CA:60:A:H5'      | 2.21                     | 0.71              |
| 1:CA:743:U:H2'     | 1:CA:744:C:C6      | 2.24                     | 0.71              |
| 1:CA:1206:G:H4'    | 3:CC:192:THR:O     | 1.90                     | 0.71              |
| 13:CM:50:GLU:O     | 13:CM:54:VAL:HG23  | 1.90                     | 0.71              |
| 20:CT:100:ILE:HD12 | 20:CT:100:ILE:N    | 2.06                     | 0.71              |
| 50:D1:86:SER:O     | 50:D1:90:ILE:HG13  | 1.91                     | 0.71              |
| 27:DA:1772:G:N2    | 27:DA:1774:C:H5''  | 2.05                     | 0.71              |
| 27:DA:1922:G:H2'   | 27:DA:1923:U:C6    | 2.26                     | 0.71              |
| 27:DA:2491:U:O2'   | 27:DA:2492:U:H5'   | 1.90                     | 0.71              |
| 27:DA:662:G:H2'    | 27:DA:663:G:H8     | 1.56                     | 0.71              |
| 31:DE:70:ALA:O     | 31:DE:72:VAL:N     | 2.24                     | 0.71              |
| 37:DO:16:ALA:HB2   | 37:DO:52:VAL:CG1   | 2.20                     | 0.71              |
| 39:DQ:16:ARG:O     | 39:DQ:17:LEU:HD23  | 1.89                     | 0.71              |
| 42:DT:30:VAL:HA    | 42:DT:44:ASP:HA    | 1.70                     | 0.71              |
| 44:DV:47:VAL:HG12  | 44:DV:52:VAL:HB    | 1.71                     | 0.71              |
| 47:DY:86:ARG:NH1   | 47:DY:95:LYS:HE3   | 2.05                     | 0.71              |
| 1:AA:1043:C:H2'    | 1:AA:1044:A:C8     | 2.26                     | 0.71              |
| 2:AB:57:PHE:CD2    | 2:AB:185:ILE:HD11  | 2.26                     | 0.71              |
| 4:AD:12:CYS:SG     | 4:AD:19:LEU:O      | 2.49                     | 0.71              |
| 38:BP:65:ARG:HH22  | 57:B8:15:LYS:HB2   | 1.53                     | 0.71              |
| 27:BA:1862:G:O2'   | 27:BA:1863:G:H5'   | 1.90                     | 0.71              |
| 27:BA:2006:C:H5'   | 27:BA:2006:C:H6    | 1.56                     | 0.71              |
| 27:BA:2553:G:H3'   | 27:BA:2554:U:H5''  | 1.71                     | 0.71              |
| 27:BA:2712:U:O2'   | 27:BA:2713:A:H5'   | 1.90                     | 0.71              |
| 31:BE:51:PHE:O     | 31:BE:74:PRO:HB2   | 1.89                     | 0.71              |
| 33:BG:45:GLU:OE1   | 33:BG:45:GLU:HA    | 1.89                     | 0.71              |
| 34:BH:10:PRO:HG2   | 34:BH:49:VAL:HB    | 1.72                     | 0.71              |
| 37:BO:71:ARG:HH12  | 42:BT:74:ARG:HH22  | 1.36                     | 0.71              |
| 40:BR:100:LEU:CD2  | 40:BR:113:LEU:HD13 | 2.13                     | 0.71              |
| 39:BQ:141:GLN:OXT  | 48:BZ:98:TYR:HB2   | 1.91                     | 0.71              |
| 1:CA:1028:C:H42    | 1:CA:1034:G:H21    | 1.36                     | 0.71              |
| 1:CA:701:C:H1'     | 1:CA:703:G:C2      | 2.26                     | 0.71              |
| 2:CB:91:PRO:HG3    | 2:CB:154:LEU:CB    | 2.14                     | 0.71              |
| 27:DA:107:C:H2'    | 27:DA:108:U:C6     | 2.24                     | 0.71              |
| 27:DA:1793:C:H2'   | 27:DA:1794:U:C6    | 2.25                     | 0.71              |
| 27:DA:1910:G:O2'   | 27:DA:1911:U:H5'   | 1.89                     | 0.71              |
| 27:DA:2291:U:H2'   | 27:DA:2292:C:C6    | 2.26                     | 0.71              |
| 27:DA:2362:G:C2'   | 27:DA:2363:C:H5'   | 2.21                     | 0.71              |
| 27:DA:2576:G:H8    | 27:DA:2581:G:O6    | 1.74                     | 0.71              |
| 27:DA:2745:C:H2'   | 27:DA:2746:U:C6    | 2.26                     | 0.71              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:2807:G:H3'   | 27:DA:2808:U:H5'' | 1.72                     | 0.71              |
| 27:DA:674:G:P      | 32:DF:54:ARG:HH22 | 2.13                     | 0.71              |
| 31:DE:2:LYS:O      | 31:DE:199:ARG:HA  | 1.91                     | 0.71              |
| 32:DF:2:LYS:HG2    | 32:DF:25:PRO:HB2  | 1.73                     | 0.71              |
| 34:DH:43:VAL:HG12  | 34:DH:53:GLU:HG2  | 1.70                     | 0.71              |
| 36:DN:15:LEU:HD22  | 36:DN:16:ILE:H    | 1.55                     | 0.71              |
| 37:DO:2:ILE:CG2    | 37:DO:8:LEU:HD11  | 2.21                     | 0.71              |
| 42:DT:92:GLY:O     | 42:DT:93:ARG:HB3  | 1.89                     | 0.71              |
| 46:DX:65:ARG:HD3   | 46:DX:70:LEU:CD1  | 2.19                     | 0.71              |
| 11:AK:31:THR:HA    | 11:AK:42:TRP:HA   | 1.72                     | 0.71              |
| 27:BA:2305:A:H5''  | 33:BG:134:GLY:HA3 | 1.72                     | 0.71              |
| 27:BA:2689:U:H5''  | 27:BA:2690:C:H5'  | 1.72                     | 0.71              |
| 27:BA:319:C:O2'    | 27:BA:320:A:H5'   | 1.91                     | 0.71              |
| 27:BA:380:U:H2'    | 27:BA:381:G:H8    | 1.55                     | 0.71              |
| 27:BA:380:U:H2'    | 27:BA:381:G:C8    | 2.26                     | 0.71              |
| 36:BN:4:TYR:HB2    | 43:BU:64:ARG:NH1  | 2.06                     | 0.71              |
| 47:BY:46:LYS:CB    | 47:BY:62:GLU:HG2  | 2.13                     | 0.71              |
| 1:CA:422:C:H4'     | 1:CA:423:G:H5''   | 1.71                     | 0.71              |
| 1:CA:475:G:H2'     | 1:CA:476:G:H8     | 1.56                     | 0.71              |
| 1:CA:601:C:H2'     | 1:CA:602:A:C8     | 2.23                     | 0.71              |
| 27:DA:422:A:H2'    | 27:DA:423:A:C8    | 2.26                     | 0.71              |
| 27:DA:479:A:H4'    | 27:DA:480:A:C5'   | 2.21                     | 0.71              |
| 27:DA:612:C:O2'    | 27:DA:613:G:H5'   | 1.91                     | 0.71              |
| 27:DA:2579:C:O2'   | 31:DE:131:ALA:HB3 | 1.90                     | 0.71              |
| 27:DA:2561:A:H4'   | 37:DO:40:VAL:HG11 | 1.73                     | 0.71              |
| 38:DP:6:LEU:HG     | 38:DP:9:ASN:CG    | 2.10                     | 0.71              |
| 39:DQ:101:ARG:HD2  | 39:DQ:102:VAL:N   | 2.06                     | 0.71              |
| 39:DQ:16:ARG:HG2   | 39:DQ:17:LEU:N    | 2.02                     | 0.71              |
| 46:DX:56:THR:O     | 46:DX:57:LEU:HB3  | 1.90                     | 0.71              |
| 48:DZ:149:LEU:HD23 | 48:DZ:170:ILE:CG1 | 2.16                     | 0.71              |
| 1:AA:628:G:O2'     | 1:AA:629:G:H5'    | 1.91                     | 0.70              |
| 5:AE:141:GLN:HA    | 5:AE:143:ARG:HH21 | 1.54                     | 0.70              |
| 11:AK:109:VAL:HG12 | 11:AK:110:ASP:H   | 1.56                     | 0.70              |
| 12:AL:119:THR:HG22 | 12:AL:120:LYS:N   | 2.05                     | 0.70              |
| 55:B6:18:ARG:HB2   | 55:B6:19:ARG:HD2  | 1.73                     | 0.70              |
| 27:BA:2884:U:H3    | 54:B5:51:TYR:HE1  | 1.37                     | 0.70              |
| 31:BE:8:LYS:HE3    | 31:BE:188:VAL:CG1 | 2.20                     | 0.70              |
| 39:BQ:16:ARG:HG2   | 39:BQ:17:LEU:N    | 2.04                     | 0.70              |
| 42:BT:23:ARG:O     | 42:BT:25:GLY:N    | 2.22                     | 0.70              |
| 43:BU:90:VAL:HG12  | 43:BU:91:ASP:N    | 2.02                     | 0.70              |
| 46:BX:30:VAL:CG2   | 46:BX:39:ILE:HD11 | 2.14                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1327:C:O2'    | 1:CA:1328:C:H5'    | 1.90                     | 0.70              |
| 1:CA:1356:G:H1     | 1:CA:1366:C:N4     | 1.88                     | 0.70              |
| 1:CA:320:C:H1'     | 1:CA:1434:A:H2     | 1.55                     | 0.70              |
| 4:CD:33:MET:HE2    | 4:CD:37:PRO:HA     | 1.73                     | 0.70              |
| 9:CI:65:VAL:HG21   | 9:CI:73:GLN:HB3    | 1.73                     | 0.70              |
| 10:CJ:48:THR:HA    | 10:CJ:62:HIS:CB    | 2.21                     | 0.70              |
| 53:D4:46:ASN:ND2   | 53:D4:47:VAL:H     | 1.89                     | 0.70              |
| 56:D7:5:TRP:CZ2    | 56:D7:7:PRO:HB3    | 2.26                     | 0.70              |
| 27:DA:1548:C:H2'   | 27:DA:1549:C:H6    | 1.55                     | 0.70              |
| 27:DA:2683:C:H2'   | 27:DA:2684:U:H6    | 1.56                     | 0.70              |
| 27:DA:271(D):G:H1  | 27:DA:271(T):C:H42 | 1.39                     | 0.70              |
| 37:DO:63:VAL:HG23  | 37:DO:64:ARG:HG3   | 1.71                     | 0.70              |
| 45:DW:83:LYS:HG2   | 45:DW:97:LYS:HD3   | 1.72                     | 0.70              |
| 48:DZ:96:GLU:HB3   | 48:DZ:124:LEU:HD11 | 1.71                     | 0.70              |
| 4:AD:70:ILE:HG23   | 4:AD:71:SER:O      | 1.90                     | 0.70              |
| 5:AE:41:VAL:CG1    | 5:AE:113:ALA:HA    | 2.21                     | 0.70              |
| 14:AN:26:ARG:CZ    | 14:AN:47:LEU:HD21  | 2.21                     | 0.70              |
| 20:AT:87:LYS:O     | 20:AT:91:LEU:HG    | 1.90                     | 0.70              |
| 27:BA:2239:G:H2'   | 27:BA:2240:C:C6    | 2.26                     | 0.70              |
| 27:BA:246:C:H41    | 57:B8:8:LYS:HG2    | 1.54                     | 0.70              |
| 32:BF:160:ASN:HD21 | 32:BF:162:LEU:HB2  | 1.55                     | 0.70              |
| 36:BN:13:TRP:O     | 36:BN:135:PRO:HD2  | 1.90                     | 0.70              |
| 38:BP:144:GLU:N    | 38:BP:145:PRO:HD3  | 2.06                     | 0.70              |
| 27:BA:911:A:H2'    | 39:BQ:9:TYR:OH     | 1.90                     | 0.70              |
| 1:CA:54:C:N4       | 1:CA:352:C:H2'     | 2.06                     | 0.70              |
| 1:CA:637:G:H2'     | 1:CA:638:G:H8      | 1.54                     | 0.70              |
| 1:CA:961:U:HO2'    | 1:CA:962:C:H6      | 1.39                     | 0.70              |
| 2:CB:174:VAL:HG13  | 2:CB:184:VAL:HG21  | 1.73                     | 0.70              |
| 4:CD:9:CYS:SG      | 60:CD:301:ZN:ZN    | 1.79                     | 0.70              |
| 5:CE:80:ILE:HD11   | 5:CE:91:LEU:HB2    | 1.73                     | 0.70              |
| 17:CQ:52:LYS:HG2   | 17:CQ:55:ASP:OD2   | 1.91                     | 0.70              |
| 49:D0:29:GLN:O     | 49:D0:67:VAL:HG23  | 1.90                     | 0.70              |
| 58:D9:17:ILE:HG22  | 58:D9:19:ARG:HG2   | 1.72                     | 0.70              |
| 27:DA:1287:A:N6    | 27:DA:1649:G:H1'   | 2.05                     | 0.70              |
| 27:DA:226:G:O2'    | 27:DA:227:A:H8     | 1.74                     | 0.70              |
| 27:DA:2562:U:H1'   | 37:DO:23:ARG:NH1   | 2.05                     | 0.70              |
| 27:DA:39:C:O2'     | 27:DA:40:C:H5'     | 1.90                     | 0.70              |
| 27:DA:616:G:H4'    | 32:DF:205:ARG:HD2  | 1.71                     | 0.70              |
| 27:DA:851:U:H4'    | 52:D3:45:GLY:O     | 1.91                     | 0.70              |
| 32:DF:1:MET:SD     | 32:DF:26:ALA:HA    | 2.31                     | 0.70              |
| 34:DH:12:PRO:O     | 34:DH:13:LYS:HB2   | 1.90                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DP:84:ASN:HA    | 38:DP:115:LEU:O    | 1.90                     | 0.70              |
| 42:DT:42:ILE:H     | 42:DT:42:ILE:CD1   | 1.92                     | 0.70              |
| 45:DW:4:LYS:HG2    | 45:DW:106:ILE:CG2  | 2.21                     | 0.70              |
| 1:AA:1248:A:H2'    | 1:AA:1249:C:H5'    | 1.73                     | 0.70              |
| 1:AA:254:G:H1      | 1:AA:272:C:H42     | 1.37                     | 0.70              |
| 1:AA:820:U:H4'     | 1:AA:821:G:OP2     | 1.90                     | 0.70              |
| 8:AH:83:ILE:HB     | 8:AH:137:VAL:HG13  | 1.72                     | 0.70              |
| 45:BW:38:TYR:OH    | 54:B5:47:PRO:HG3   | 1.91                     | 0.70              |
| 58:B9:26:ILE:HD12  | 58:B9:26:ILE:N     | 2.06                     | 0.70              |
| 27:BA:1208:C:H5'   | 27:BA:1209:G:OP2   | 1.91                     | 0.70              |
| 27:BA:1722:A:O2'   | 27:BA:1739:U:H5''  | 1.90                     | 0.70              |
| 27:BA:2305:A:H61   | 33:BG:43:LEU:H     | 1.40                     | 0.70              |
| 30:BD:108:PRO:HG3  | 30:BD:143:HIS:CE1  | 2.25                     | 0.70              |
| 39:BQ:133:ARG:O    | 39:BQ:134:ARG:HB2  | 1.91                     | 0.70              |
| 43:BU:90:VAL:HG11  | 44:BV:40:LEU:HD23  | 1.71                     | 0.70              |
| 1:CA:9:G:O2'       | 1:CA:10:A:H8       | 1.74                     | 0.70              |
| 1:CA:1324:A:H4'    | 1:CA:1362:C:H4'    | 1.73                     | 0.70              |
| 1:CA:718:G:H5'     | 11:CK:117:ASN:OD1  | 1.91                     | 0.70              |
| 11:CK:21:ILE:HB    | 11:CK:84:VAL:HG12  | 1.71                     | 0.70              |
| 49:D0:17:GLN:O     | 49:D0:19:LYS:HD3   | 1.91                     | 0.70              |
| 27:DA:1992:G:O2'   | 27:DA:1993:U:OP2   | 2.06                     | 0.70              |
| 27:DA:2086:U:H2'   | 27:DA:2087:G:H8    | 1.56                     | 0.70              |
| 27:DA:2134:A:N6    | 27:DA:2157:G:H1'   | 2.06                     | 0.70              |
| 27:DA:90:U:H1'     | 27:DA:92:A:C8      | 2.26                     | 0.70              |
| 29:DC:68:LEU:HB3   | 29:DC:70:LYS:HE2   | 1.74                     | 0.70              |
| 33:DG:115:ARG:HH12 | 33:DG:136:ARG:HH11 | 1.39                     | 0.70              |
| 33:DG:36:LYS:HG2   | 33:DG:160:VAL:HG21 | 1.73                     | 0.70              |
| 37:DO:86:ILE:H     | 37:DO:86:ILE:HD12  | 1.56                     | 0.70              |
| 41:DS:92:TYR:CG    | 41:DS:93:LYS:N     | 2.54                     | 0.70              |
| 4:AD:172:PRO:HG2   | 4:AD:193:ASP:OD1   | 1.90                     | 0.70              |
| 5:AE:40:ARG:HB3    | 5:AE:66:MET:CE     | 2.21                     | 0.70              |
| 5:AE:78:HIS:HE1    | 5:AE:142:LEU:HA    | 1.55                     | 0.70              |
| 10:AJ:5:ARG:HG3    | 10:AJ:73:ASP:OD1   | 1.91                     | 0.70              |
| 10:AJ:4:ILE:O      | 10:AJ:74:ILE:HG12  | 1.90                     | 0.70              |
| 27:BA:143:G:H5''   | 27:BA:1598:C:O2'   | 1.91                     | 0.70              |
| 27:BA:1885:A:H2'   | 27:BA:1886:C:O4'   | 1.91                     | 0.70              |
| 27:BA:225:A:C2'    | 27:BA:226:G:H5'    | 2.21                     | 0.70              |
| 27:BA:2562:U:C2'   | 27:BA:2563:U:H5'   | 2.22                     | 0.70              |
| 35:BI:91:SER:O     | 35:BI:92:VAL:HB    | 1.91                     | 0.70              |
| 38:BP:92:GLU:HA    | 38:BP:123:LEU:HD23 | 1.71                     | 0.70              |
| 42:BT:51:ARG:CG    | 42:BT:98:LYS:HG3   | 2.22                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BV:1:MET:HE3    | 44:BV:43:GLU:HG2   | 1.73                     | 0.70              |
| 47:BY:28:LYS:HB2   | 47:BY:37:VAL:HB    | 1.73                     | 0.70              |
| 47:BY:7:VAL:HB     | 47:BY:8:LYS:NZ     | 2.04                     | 0.70              |
| 1:CA:1010:G:H2'    | 1:CA:1011:G:C8     | 2.26                     | 0.70              |
| 1:CA:276:G:O2'     | 1:CA:277:C:H5'     | 1.91                     | 0.70              |
| 1:CA:966:G:O2'     | 1:CA:967:C:C6      | 2.44                     | 0.70              |
| 2:CB:11:LEU:CD1    | 2:CB:217:ARG:HH21  | 2.04                     | 0.70              |
| 4:CD:9:CYS:HB2     | 4:CD:22:LYS:HZ3    | 1.55                     | 0.70              |
| 7:CG:145:ALA:O     | 7:CG:146:GLU:HB2   | 1.91                     | 0.70              |
| 11:CK:103:LEU:HD13 | 11:CK:104:GLN:H    | 1.56                     | 0.70              |
| 1:CA:186:C:O3'     | 20:CT:82:SER:HB2   | 1.91                     | 0.70              |
| 50:D1:52:ARG:CG    | 50:D1:53:VAL:H     | 2.02                     | 0.70              |
| 57:D8:14:VAL:HG21  | 57:D8:22:VAL:CG1   | 2.22                     | 0.70              |
| 27:DA:1356:G:H2'   | 27:DA:1357:U:H6    | 1.56                     | 0.70              |
| 27:DA:2146:C:H5'   | 27:DA:2147:G:C4    | 2.27                     | 0.70              |
| 27:DA:373:U:H2'    | 27:DA:374:A:C8     | 2.19                     | 0.70              |
| 27:DA:903:C:H2'    | 27:DA:904:C:C6     | 2.26                     | 0.70              |
| 29:DC:188:ASN:O    | 29:DC:191:ALA:HB3  | 1.90                     | 0.70              |
| 31:DE:13:ARG:HB2   | 31:DE:21:VAL:O     | 1.91                     | 0.70              |
| 27:DA:811:U:OP2    | 38:DP:24:GLY:HA2   | 1.92                     | 0.70              |
| 38:DP:90:ARG:HB3   | 38:DP:91:PHE:CD1   | 2.26                     | 0.70              |
| 1:AA:52:G:HO2'     | 1:AA:53:A:H8       | 1.35                     | 0.70              |
| 3:AC:87:LEU:O      | 3:AC:91:LEU:HG     | 1.91                     | 0.70              |
| 4:AD:54:TYR:CE1    | 4:AD:209:ARG:HD2   | 2.26                     | 0.70              |
| 5:AE:33:VAL:HG12   | 5:AE:112:LEU:HD12  | 1.74                     | 0.70              |
| 12:AL:80:VAL:HG11  | 12:AL:104:ALA:HB3  | 1.74                     | 0.70              |
| 27:BA:2629:A:N3    | 27:BA:2629:A:H2'   | 2.05                     | 0.70              |
| 31:BE:105:THR:HG21 | 31:BE:164:ARG:NH1  | 2.04                     | 0.70              |
| 34:BH:22:GLY:O     | 34:BH:36:PRO:HA    | 1.91                     | 0.70              |
| 34:BH:29:PRO:O     | 34:BH:30:LYS:HE3   | 1.90                     | 0.70              |
| 38:BP:122:PRO:HB3  | 38:BP:141:ALA:CB   | 2.20                     | 0.70              |
| 39:BQ:115:MET:HE2  | 39:BQ:131:ILE:HG21 | 1.74                     | 0.70              |
| 44:BV:22:VAL:HG21  | 44:BV:94:LEU:HD11  | 1.73                     | 0.70              |
| 1:CA:232:G:H2'     | 1:CA:233:C:H6      | 1.57                     | 0.70              |
| 1:CA:977:A:N3      | 1:CA:977:A:H2'     | 2.05                     | 0.70              |
| 3:CC:123:GLN:O     | 3:CC:128:PHE:HB2   | 1.91                     | 0.70              |
| 11:CK:29:ILE:HD12  | 11:CK:43:SER:O     | 1.92                     | 0.70              |
| 12:CL:15:VAL:HG23  | 12:CL:16:ARG:N     | 2.03                     | 0.70              |
| 27:DA:2569:G:O2'   | 27:DA:2570:G:H5'   | 1.92                     | 0.70              |
| 27:DA:2875:C:H4'   | 42:DT:5:ALA:CB     | 2.21                     | 0.70              |
| 30:DD:69:ARG:NH1   | 30:DD:130:ALA:HB2  | 2.07                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DE:111:ARG:HD2 | 31:DE:160:TYR:CD1  | 2.26                     | 0.70              |
| 44:DV:38:LEU:HD12 | 44:DV:56:SER:N     | 2.06                     | 0.70              |
| 1:AA:1118:C:H2'   | 1:AA:1119:C:C6     | 2.26                     | 0.70              |
| 1:AA:257:G:H2'    | 1:AA:258:G:C8      | 2.26                     | 0.70              |
| 1:AA:486:U:H6     | 1:AA:486:U:H5'     | 1.56                     | 0.70              |
| 17:AQ:8:GLY:HA3   | 17:AQ:22:LEU:O     | 1.92                     | 0.70              |
| 27:BA:105:C:O2    | 27:BA:105:C:H2'    | 1.90                     | 0.70              |
| 27:BA:1879:C:C2'  | 27:BA:1880:C:H5''  | 2.21                     | 0.70              |
| 27:BA:2299:G:N1   | 27:BA:2318:G:C8    | 2.60                     | 0.70              |
| 27:BA:2466:C:O2'  | 27:BA:2467:C:H5'   | 1.90                     | 0.70              |
| 27:BA:2732:G:H3'  | 27:BA:2733:A:C5'   | 2.21                     | 0.70              |
| 27:BA:45:C:OP2    | 27:BA:215:G:H5''   | 1.91                     | 0.70              |
| 27:BA:466:A:N3    | 27:BA:683:C:H1'    | 2.06                     | 0.70              |
| 27:BA:81:G:H1     | 27:BA:105:C:H42    | 1.37                     | 0.70              |
| 27:BA:965:C:H2'   | 27:BA:966:G:H8     | 1.57                     | 0.70              |
| 35:BI:83:ALA:HB2  | 35:BI:88:ILE:HG23  | 1.73                     | 0.70              |
| 37:BO:11:ALA:O    | 37:BO:98:VAL:HA    | 1.91                     | 0.70              |
| 38:BP:105:LEU:N   | 38:BP:105:LEU:HD23 | 2.07                     | 0.70              |
| 44:BV:87:HIS:NE2  | 44:BV:89:GLN:HG2   | 2.05                     | 0.70              |
| 2:CB:187:LEU:HB2  | 2:CB:201:ILE:HB    | 1.74                     | 0.70              |
| 7:CG:87:VAL:HG11  | 7:CG:154:TYR:O     | 1.91                     | 0.70              |
| 12:CL:107:VAL:CG1 | 12:CL:110:ARG:HB2  | 2.22                     | 0.70              |
| 13:CM:3:ARG:HG2   | 13:CM:9:ILE:HG12   | 1.70                     | 0.70              |
| 17:CQ:78:GLU:OE1  | 17:CQ:81:ARG:HD2   | 1.92                     | 0.70              |
| 51:D2:18:PRO:HG2  | 51:D2:19:VAL:H     | 1.55                     | 0.70              |
| 27:DA:1162:G:O2'  | 27:DA:1163:G:H5'   | 1.92                     | 0.70              |
| 27:DA:1233:C:H2'  | 27:DA:1234:U:H6    | 1.56                     | 0.70              |
| 27:DA:1799:G:H5'  | 27:DA:1819:A:N6    | 2.06                     | 0.70              |
| 27:DA:2100:G:H1   | 27:DA:2189:U:H3    | 1.38                     | 0.70              |
| 27:DA:630:G:H1    | 27:DA:634:C:H42    | 1.38                     | 0.70              |
| 31:DE:16:ARG:O    | 31:DE:17:ASP:HB2   | 1.91                     | 0.70              |
| 32:DF:25:PRO:CG   | 32:DF:119:ARG:HB2  | 2.21                     | 0.70              |
| 36:DN:46:VAL:O    | 36:DN:47:ALA:HB3   | 1.91                     | 0.70              |
| 38:DP:136:GLU:O   | 38:DP:139:LYS:N    | 2.25                     | 0.70              |
| 42:DT:13:ARG:CZ   | 42:DT:13:ARG:HA    | 2.21                     | 0.70              |
| 48:DZ:9:ARG:H     | 48:DZ:36:VAL:HA    | 1.56                     | 0.70              |
| 1:AA:592:G:C2     | 1:AA:648:A:C2      | 2.79                     | 0.70              |
| 1:AA:579:G:H5'    | 1:AA:728:A:H1'     | 1.71                     | 0.70              |
| 1:AA:807:A:O2'    | 1:AA:808:C:H5'     | 1.91                     | 0.70              |
| 6:AF:9:VAL:HG12   | 6:AF:86:ARG:HB2    | 1.72                     | 0.70              |
| 15:AO:78:TYR:O    | 15:AO:82:ILE:HG22  | 1.92                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 57:B8:29:LYS:HD3  | 57:B8:44:LYS:HG2  | 1.71                     | 0.70              |
| 27:BA:1481:U:H2'  | 27:BA:1481:U:O2   | 1.91                     | 0.70              |
| 28:BB:87:G:C3'    | 28:BB:88:C:H5''   | 2.22                     | 0.70              |
| 36:BN:115:ARG:O   | 36:BN:118:LYS:HB2 | 1.91                     | 0.70              |
| 37:BO:110:GLY:HA2 | 37:BO:112:MET:CE  | 2.20                     | 0.70              |
| 38:BP:6:LEU:H     | 38:BP:6:LEU:HD23  | 1.56                     | 0.70              |
| 28:BB:7:G:H21     | 41:BS:38:GLN:HE22 | 1.40                     | 0.70              |
| 44:BV:99:ILE:O    | 44:BV:99:ILE:HG12 | 1.90                     | 0.70              |
| 1:CA:532:A:H62    | 3:CC:156:ARG:HH12 | 1.38                     | 0.70              |
| 27:DA:1681:G:C8   | 27:DA:1681:G:OP2  | 2.42                     | 0.70              |
| 27:DA:2158:A:H4'  | 27:DA:2159:G:O5'  | 1.90                     | 0.70              |
| 27:DA:2304:G:H5'' | 27:DA:2305:A:OP2  | 1.92                     | 0.70              |
| 27:DA:2466:C:C2'  | 27:DA:2467:C:H5'  | 2.21                     | 0.70              |
| 27:DA:2523:G:H5'  | 27:DA:2523:G:H8   | 1.57                     | 0.70              |
| 27:DA:2590:A:O2'  | 27:DA:2591:C:H5'  | 1.92                     | 0.70              |
| 27:DA:706:A:OP1   | 30:DD:7:LYS:HE3   | 1.91                     | 0.70              |
| 30:DD:26:LYS:HZ1  | 30:DD:82:ILE:H    | 1.39                     | 0.70              |
| 31:DE:9:VAL:HG13  | 31:DE:25:VAL:HB   | 1.74                     | 0.70              |
| 32:DF:7:TYR:O     | 32:DF:8:GLN:HB2   | 1.90                     | 0.70              |
| 37:DO:53:LYS:N    | 37:DO:53:LYS:HD2  | 2.06                     | 0.70              |
| 1:AA:1206:G:H2'   | 1:AA:1207:G:H5'   | 1.73                     | 0.70              |
| 10:AJ:6:ILE:HA    | 10:AJ:97:GLU:O    | 1.91                     | 0.70              |
| 58:B9:29:ASN:HD21 | 58:B9:32:HIS:CE1  | 2.09                     | 0.70              |
| 27:BA:1400:G:H2'  | 27:BA:1401:G:C8   | 2.25                     | 0.70              |
| 27:BA:1591:G:H2'  | 27:BA:1592:C:H6   | 1.57                     | 0.70              |
| 27:BA:1669:A:H2'  | 27:BA:1670:C:H5'  | 1.72                     | 0.70              |
| 27:BA:2071:A:C2   | 27:BA:2441:C:N3   | 2.57                     | 0.70              |
| 27:BA:327:G:H2'   | 27:BA:328:U:C6    | 2.27                     | 0.70              |
| 31:BE:36:ARG:HH22 | 31:BE:88:GLY:HA3  | 1.55                     | 0.70              |
| 37:BO:103:ALA:C   | 37:BO:105:GLU:H   | 1.94                     | 0.70              |
| 40:BR:37:THR:OG1  | 40:BR:39:PRO:HD2  | 1.92                     | 0.70              |
| 41:BS:17:ARG:HA   | 41:BS:20:ARG:HH11 | 1.55                     | 0.70              |
| 42:BT:127:ALA:C   | 42:BT:129:ARG:H   | 1.95                     | 0.70              |
| 1:CA:1494:G:O6    | 26:CZ:1:KBE:HAA   | 1.91                     | 0.70              |
| 1:CA:256:U:H2'    | 1:CA:257:G:C8     | 2.26                     | 0.70              |
| 14:CN:26:ARG:NH2  | 14:CN:47:LEU:HD21 | 2.07                     | 0.70              |
| 33:DG:2:PRO:HD2   | 53:D4:51:TYR:CE2  | 2.26                     | 0.70              |
| 27:DA:1952:A:C2   | 37:DO:22:ILE:HG23 | 2.27                     | 0.70              |
| 27:DA:2019:A:H61  | 27:DA:2035:G:H1   | 1.40                     | 0.70              |
| 27:DA:2052:G:N2   | 27:DA:2618:G:H1'  | 2.07                     | 0.70              |
| 32:DF:89:VAL:HG12 | 32:DF:90:PHE:H    | 1.57                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DH:147:ASN:O   | 34:DH:150:ALA:HB3  | 1.92                     | 0.70              |
| 1:AA:6:G:H4'      | 1:AA:298:A:H4'     | 1.74                     | 0.70              |
| 1:AA:973:G:H3'    | 1:AA:974:A:H5''    | 1.73                     | 0.70              |
| 1:AA:509:A:H5'    | 4:AD:54:TYR:CD2    | 2.27                     | 0.70              |
| 27:BA:158:U:H2'   | 27:BA:158:U:O2     | 1.92                     | 0.70              |
| 27:BA:1718:G:H8   | 27:BA:1718:G:H5'   | 1.56                     | 0.70              |
| 27:BA:2029:G:H2'  | 27:BA:2031:A:OP1   | 1.92                     | 0.70              |
| 27:BA:335:C:H2'   | 27:BA:336:C:H6     | 1.56                     | 0.70              |
| 27:BA:598:G:H5'   | 38:BP:15:ARG:HG3   | 1.73                     | 0.70              |
| 27:BA:838:C:H2'   | 27:BA:839:U:H6     | 1.56                     | 0.70              |
| 30:BD:112:GLN:HB2 | 30:BD:115:GLN:HE21 | 1.57                     | 0.70              |
| 31:BE:119:ARG:HD2 | 31:BE:120:TRP:NE1  | 2.07                     | 0.70              |
| 32:BF:65:TRP:CH2  | 32:BF:75:HIS:HD2   | 2.08                     | 0.70              |
| 42:BT:31:SER:OG   | 42:BT:32:TYR:N     | 2.25                     | 0.70              |
| 27:BA:2875:C:C4'  | 42:BT:5:ALA:HB2    | 2.21                     | 0.70              |
| 1:CA:457:C:H2'    | 1:CA:458:C:H6      | 1.57                     | 0.70              |
| 1:CA:686:U:H3     | 1:CA:703:G:H21     | 1.39                     | 0.70              |
| 1:CA:913:A:H4'    | 1:CA:914:A:O5'     | 1.90                     | 0.70              |
| 2:CB:200:ILE:HG22 | 2:CB:202:PRO:HD3   | 1.74                     | 0.70              |
| 3:CC:153:VAL:HG12 | 3:CC:196:LEU:CD1   | 2.21                     | 0.70              |
| 7:CG:40:ALA:HB1   | 9:CI:41:VAL:HG11   | 1.74                     | 0.70              |
| 17:CQ:21:VAL:O    | 17:CQ:41:LYS:HA    | 1.92                     | 0.70              |
| 27:DA:2832:U:H4'  | 27:DA:2833:G:H5''  | 1.71                     | 0.70              |
| 27:DA:754:C:H2'   | 27:DA:755:C:H6     | 1.52                     | 0.70              |
| 40:DR:10:LEU:CD2  | 40:DR:17:ARG:HD2   | 2.21                     | 0.70              |
| 37:DO:119:PRO:HB2 | 42:DT:68:TYR:CE1   | 2.26                     | 0.70              |
| 46:DX:66:LEU:O    | 46:DX:66:LEU:HD23  | 1.91                     | 0.70              |
| 1:AA:1096:C:H2'   | 1:AA:1097:C:H6     | 1.55                     | 0.70              |
| 1:AA:960:U:O2'    | 1:AA:1223:C:H5'    | 1.91                     | 0.70              |
| 3:AC:14:ILE:CD1   | 3:AC:178:LEU:HB3   | 2.22                     | 0.70              |
| 15:AO:9:GLN:HA    | 15:AO:12:ILE:HD12  | 1.73                     | 0.70              |
| 27:BA:1414:G:H1   | 27:BA:1588:C:N4    | 1.87                     | 0.70              |
| 27:BA:2758:A:H2'  | 27:BA:2759:G:H5'   | 1.74                     | 0.70              |
| 30:BD:35:LYS:HA   | 30:BD:64:ILE:HG22  | 1.74                     | 0.70              |
| 31:BE:108:SER:O   | 31:BE:162:ALA:HA   | 1.92                     | 0.70              |
| 27:BA:2580:U:H5'  | 31:BE:131:ALA:HB3  | 1.74                     | 0.70              |
| 39:BQ:38:GLU:OE2  | 39:BQ:128:LYS:HG2  | 1.91                     | 0.70              |
| 42:BT:92:GLY:HA2  | 42:BT:114:LEU:HD22 | 1.74                     | 0.70              |
| 43:BU:25:TRP:CD1  | 43:BU:26:GLY:N     | 2.60                     | 0.70              |
| 48:BZ:150:HIS:HB3 | 48:BZ:169:THR:HA   | 1.72                     | 0.70              |
| 1:CA:1106:G:H2'   | 1:CA:1107:C:H6     | 1.57                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1406:U:H2'   | 1:CA:1407:C:H6    | 1.56                     | 0.70              |
| 13:CM:90:LEU:HA   | 13:CM:93:ARG:HB2  | 1.74                     | 0.70              |
| 27:DA:1602:U:H3'  | 27:DA:1603:A:C5'  | 2.21                     | 0.70              |
| 27:DA:2223:G:C2'  | 27:DA:2224:G:H5'  | 2.22                     | 0.70              |
| 27:DA:286:C:H2'   | 27:DA:286:C:O2    | 1.91                     | 0.70              |
| 27:DA:597:U:H2'   | 27:DA:598:G:C8    | 2.27                     | 0.70              |
| 38:DP:59:LEU:CA   | 38:DP:61:ARG:CZ   | 2.68                     | 0.70              |
| 41:DS:78:LEU:HD11 | 41:DS:103:GLU:HB3 | 1.72                     | 0.70              |
| 48:DZ:128:SER:HB3 | 48:DZ:131:ASN:ND2 | 2.07                     | 0.70              |
| 1:AA:1236:A:H2'   | 1:AA:1237:C:C6    | 2.27                     | 0.69              |
| 1:AA:197:A:H4'    | 1:AA:198:G:OP1    | 1.92                     | 0.69              |
| 1:AA:35:G:O2'     | 1:AA:36:C:H5'     | 1.91                     | 0.69              |
| 1:AA:453:A:H2'    | 1:AA:454:C:C6     | 2.27                     | 0.69              |
| 1:AA:472:A:C2     | 1:AA:473:G:H1'    | 2.26                     | 0.69              |
| 4:AD:114:ARG:O    | 4:AD:118:ARG:HB2  | 1.92                     | 0.69              |
| 19:AS:63:THR:HG22 | 19:AS:66:MET:HE3  | 1.73                     | 0.69              |
| 27:BA:1141:U:OP1  | 36:BN:25:ARG:NH1  | 2.25                     | 0.69              |
| 27:BA:1193:G:H8   | 27:BA:1193:G:H5'  | 1.57                     | 0.69              |
| 27:BA:1579:A:H2'  | 27:BA:1580:A:C8   | 2.27                     | 0.69              |
| 27:BA:436:C:H2'   | 27:BA:437:G:H8    | 1.57                     | 0.69              |
| 27:BA:469:G:C2'   | 27:BA:470:A:H5''  | 2.21                     | 0.69              |
| 27:BA:703:U:O2'   | 27:BA:704:G:H5'   | 1.91                     | 0.69              |
| 28:BB:7:G:C3'     | 28:BB:8:U:H5''    | 2.22                     | 0.69              |
| 1:CA:1104:G:O2'   | 1:CA:1105:A:H5'   | 1.92                     | 0.69              |
| 1:CA:71:C:O2'     | 1:CA:72:C:H5'     | 1.92                     | 0.69              |
| 1:CA:978:A:O2'    | 1:CA:1322:C:N3    | 2.24                     | 0.69              |
| 10:CJ:40:LEU:HD23 | 10:CJ:40:LEU:H    | 1.57                     | 0.69              |
| 24:CX:32:C:H2'    | 24:CX:33:U:O4'    | 1.91                     | 0.69              |
| 27:DA:1127:A:H2'  | 27:DA:1128:A:H5'' | 1.73                     | 0.69              |
| 27:DA:1625:C:H2'  | 27:DA:1626:G:H5'  | 1.72                     | 0.69              |
| 27:DA:1639:U:H2'  | 27:DA:1640:C:H5'' | 1.73                     | 0.69              |
| 27:DA:1887:C:C3'  | 27:DA:1888:G:H5'' | 2.22                     | 0.69              |
| 27:DA:2453:A:H4'  | 27:DA:2572:A:O2'  | 1.91                     | 0.69              |
| 27:DA:2821:A:H2'  | 27:DA:2822:G:C8   | 2.27                     | 0.69              |
| 27:DA:414:C:H1'   | 27:DA:1864:U:O2'  | 1.92                     | 0.69              |
| 39:DQ:27:VAL:CG1  | 39:DQ:29:PHE:H    | 2.04                     | 0.69              |
| 39:DQ:51:ARG:HB3  | 39:DQ:51:ARG:HH11 | 1.55                     | 0.69              |
| 27:DA:1187:G:H5'' | 44:DV:81:TYR:CE2  | 2.27                     | 0.69              |
| 1:AA:1163:C:H2'   | 1:AA:1164:G:C8    | 2.26                     | 0.69              |
| 5:AE:57:LYS:HG2   | 5:AE:61:TYR:HE2   | 1.57                     | 0.69              |
| 53:B4:60:GLU:O    | 53:B4:61:VAL:HB   | 1.92                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:B5:2:ALA:O      | 54:B5:3:LYS:HD2    | 1.91                     | 0.69              |
| 27:BA:1495:A:H2'   | 27:BA:1496:A:C2    | 2.26                     | 0.69              |
| 27:BA:17:G:H4'     | 43:BU:25:TRP:CZ2   | 2.26                     | 0.69              |
| 32:BF:160:ASN:ND2  | 32:BF:162:LEU:H    | 1.90                     | 0.69              |
| 32:BF:164:ARG:CZ   | 32:BF:164:ARG:HB2  | 2.19                     | 0.69              |
| 34:BH:19:VAL:HB    | 34:BH:44:VAL:HG13  | 1.73                     | 0.69              |
| 35:BI:4:ILE:HD13   | 35:BI:47:LEU:HD13  | 1.74                     | 0.69              |
| 36:BN:58:ASP:O     | 36:BN:59:LYS:HB2   | 1.92                     | 0.69              |
| 46:BX:64:LYS:HZ2   | 46:BX:73:ARG:HH21  | 1.37                     | 0.69              |
| 47:BY:28:LYS:O     | 47:BY:38:ILE:HB    | 1.91                     | 0.69              |
| 1:CA:731:G:O2'     | 1:CA:732:C:H5'     | 1.91                     | 0.69              |
| 1:CA:880:C:O2'     | 1:CA:881:G:H5'     | 1.92                     | 0.69              |
| 1:CA:979:C:H3'     | 1:CA:980:C:C5'     | 2.19                     | 0.69              |
| 4:CD:131:ARG:HD3   | 4:CD:131:ARG:H     | 1.57                     | 0.69              |
| 10:CJ:40:LEU:CG    | 10:CJ:69:ASN:HB3   | 2.21                     | 0.69              |
| 1:CA:973:G:H1'     | 10:CJ:55:LYS:HE2   | 1.72                     | 0.69              |
| 27:DA:1825:A:H2'   | 27:DA:1826:G:H8    | 1.57                     | 0.69              |
| 27:DA:2482:G:H2'   | 27:DA:2483:C:H6    | 1.55                     | 0.69              |
| 27:DA:271(R):G:H2' | 27:DA:271(S):G:C8  | 2.26                     | 0.69              |
| 30:DD:267:SER:O    | 30:DD:268:ARG:HB2  | 1.91                     | 0.69              |
| 32:DF:34:TRP:CE2   | 38:DP:12:ALA:HB2   | 2.26                     | 0.69              |
| 33:DG:133:LEU:HD11 | 33:DG:157:ILE:HD11 | 1.74                     | 0.69              |
| 34:DH:117:PRO:HB3  | 34:DH:123:PHE:CE1  | 2.27                     | 0.69              |
| 36:DN:57:ALA:CB    | 36:DN:124:ALA:HA   | 2.21                     | 0.69              |
| 41:DS:85:VAL:H     | 41:DS:106:ARG:CB   | 1.99                     | 0.69              |
| 44:DV:49:THR:HG22  | 44:DV:50:PRO:HD2   | 1.74                     | 0.69              |
| 46:DX:57:LEU:HD11  | 46:DX:78:LYS:HD3   | 1.74                     | 0.69              |
| 4:AD:128:VAL:C     | 4:AD:130:GLY:H     | 1.96                     | 0.69              |
| 14:AN:6:LEU:HD13   | 14:AN:23:ARG:NH2   | 2.07                     | 0.69              |
| 20:AT:89:ARG:NH2   | 20:AT:104:LEU:HD11 | 2.07                     | 0.69              |
| 23:AW:23:G:H8      | 23:AW:23:G:H5'     | 1.57                     | 0.69              |
| 55:B6:36:LEU:HB3   | 55:B6:50:ARG:NH1   | 2.06                     | 0.69              |
| 27:BA:1754:C:H6    | 42:BT:96:ARG:NH1   | 1.89                     | 0.69              |
| 27:BA:2016:U:H2'   | 27:BA:2017:U:H6    | 1.56                     | 0.69              |
| 27:BA:517:C:O2'    | 27:BA:518:G:H5'    | 1.92                     | 0.69              |
| 32:BF:176:LEU:HD12 | 32:BF:177:ALA:H    | 1.58                     | 0.69              |
| 33:BG:15:VAL:HG21  | 33:BG:176:LEU:HG   | 1.74                     | 0.69              |
| 33:BG:28:VAL:O     | 33:BG:31:VAL:HG12  | 1.92                     | 0.69              |
| 43:BU:34:LYS:HA    | 43:BU:34:LYS:HE2   | 1.73                     | 0.69              |
| 1:CA:1275:A:H2'    | 1:CA:1276:G:C8     | 2.27                     | 0.69              |
| 1:CA:642:A:C5      | 8:CH:115:SER:HA    | 2.27                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CK:22:HIS:HB3   | 11:CK:29:ILE:CG2   | 2.20                     | 0.69              |
| 16:CP:42:ARG:HB2   | 16:CP:44:THR:HG23  | 1.72                     | 0.69              |
| 27:DA:479:A:H4'    | 27:DA:480:A:H5'    | 1.73                     | 0.69              |
| 33:DG:146:TYR:O    | 33:DG:149:VAL:HG22 | 1.92                     | 0.69              |
| 36:DN:133:GLN:CG   | 36:DN:135:PRO:HD3  | 2.21                     | 0.69              |
| 36:DN:86:PRO:HG2   | 36:DN:89:LYS:CG    | 2.22                     | 0.69              |
| 1:AA:264:U:H4'     | 17:AQ:63:ARG:HD3   | 1.75                     | 0.69              |
| 1:AA:657:G:O2'     | 1:AA:658:G:H5'     | 1.92                     | 0.69              |
| 2:AB:32:ILE:HG12   | 2:AB:33:TYR:H      | 1.58                     | 0.69              |
| 3:AC:193:TYR:CD2   | 3:AC:193:TYR:N     | 2.59                     | 0.69              |
| 9:AI:48:GLU:C      | 9:AI:50:LEU:H      | 1.96                     | 0.69              |
| 9:AI:83:ARG:O      | 9:AI:86:VAL:HG12   | 1.92                     | 0.69              |
| 17:AQ:10:VAL:HA    | 17:AQ:20:THR:O     | 1.93                     | 0.69              |
| 18:AR:73:ALA:HB3   | 18:AR:79:LEU:HD12  | 1.75                     | 0.69              |
| 58:B9:2:LYS:O      | 58:B9:2:LYS:HD3    | 1.91                     | 0.69              |
| 30:BD:112:GLN:H    | 30:BD:115:GLN:NE2  | 1.91                     | 0.69              |
| 30:BD:267:SER:C    | 30:BD:269:PHE:H    | 1.92                     | 0.69              |
| 32:BF:39:TRP:O     | 32:BF:43:LYS:HG2   | 1.92                     | 0.69              |
| 35:BI:111:PRO:CA   | 35:BI:114:LEU:HD21 | 2.22                     | 0.69              |
| 38:BP:107:LYS:C    | 38:BP:109:GLY:H    | 1.96                     | 0.69              |
| 48:BZ:60:LEU:HB2   | 48:BZ:64:GLN:HB2   | 1.74                     | 0.69              |
| 1:CA:470:C:H5''    | 1:CA:471:G:OP2     | 1.92                     | 0.69              |
| 1:CA:603:U:H2'     | 1:CA:604:G:C8      | 2.25                     | 0.69              |
| 2:CB:213:LEU:O     | 2:CB:217:ARG:HG2   | 1.93                     | 0.69              |
| 3:CC:182:ILE:HG12  | 3:CC:203:PHE:HA    | 1.72                     | 0.69              |
| 32:DF:3:GLU:HB2    | 32:DF:19:GLU:HB2   | 1.74                     | 0.69              |
| 35:DI:40:THR:O     | 35:DI:44:LEU:HB2   | 1.92                     | 0.69              |
| 41:DS:87:PHE:HB2   | 41:DS:106:ARG:NH1  | 2.07                     | 0.69              |
| 42:DT:49:VAL:C     | 42:DT:50:ILE:HD12  | 2.13                     | 0.69              |
| 44:DV:41:GLY:H     | 44:DV:45:THR:HB    | 1.56                     | 0.69              |
| 1:AA:104:G:O2'     | 1:AA:105:G:H5'     | 1.93                     | 0.69              |
| 1:AA:1112:C:H42    | 3:AC:177:THR:HA    | 1.56                     | 0.69              |
| 17:AQ:27:PHE:HD1   | 17:AQ:28:PRO:O     | 1.76                     | 0.69              |
| 27:BA:1273:U:H5''  | 27:BA:1273:U:C6    | 2.19                     | 0.69              |
| 27:BA:1956:U:C2'   | 27:BA:1957:C:H5'   | 2.21                     | 0.69              |
| 27:BA:2118:U:O2'   | 27:BA:2119:A:H5''  | 1.93                     | 0.69              |
| 27:BA:271(P):C:H2' | 27:BA:271(Q):G:O4' | 1.91                     | 0.69              |
| 27:BA:1710:C:H4'   | 27:BA:2858:C:O2    | 1.93                     | 0.69              |
| 27:BA:527:C:C5     | 27:BA:2779:U:H2'   | 2.28                     | 0.69              |
| 29:BC:100:ILE:HG22 | 29:BC:101:GLN:HG3  | 1.72                     | 0.69              |
| 30:BD:61:LEU:HB3   | 30:BD:63:ARG:NH1   | 2.07                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BG:172:LEU:O   | 33:BG:176:LEU:HD12 | 1.92                     | 0.69              |
| 38:BP:57:THR:OG1  | 38:BP:59:LEU:HB3   | 1.93                     | 0.69              |
| 40:BR:10:LEU:HB3  | 40:BR:17:ARG:CZ    | 2.23                     | 0.69              |
| 1:CA:929:G:H1     | 1:CA:1388:C:H42    | 1.36                     | 0.69              |
| 1:CA:25:C:O2'     | 1:CA:26:A:H5'      | 1.92                     | 0.69              |
| 1:CA:31:G:H5'     | 1:CA:306:G:N2      | 2.07                     | 0.69              |
| 2:CB:16:HIS:HB3   | 2:CB:210:SER:CB    | 2.21                     | 0.69              |
| 10:CJ:50:ILE:HD13 | 10:CJ:50:ILE:H     | 1.57                     | 0.69              |
| 13:CM:31:LYS:HA   | 13:CM:34:LEU:HG    | 1.74                     | 0.69              |
| 13:CM:47:ASP:O    | 13:CM:48:LEU:HB3   | 1.91                     | 0.69              |
| 13:CM:91:ARG:HB2  | 13:CM:98:VAL:HG13  | 1.74                     | 0.69              |
| 50:D1:30:VAL:O    | 50:D1:31:GLY:O     | 2.10                     | 0.69              |
| 27:DA:2351:G:O6   | 57:D8:39:LYS:HG3   | 1.92                     | 0.69              |
| 27:DA:2173:A:H2'  | 27:DA:2174:C:C6    | 2.27                     | 0.69              |
| 27:DA:2683:C:H2'  | 27:DA:2684:U:C6    | 2.28                     | 0.69              |
| 27:DA:852:G:H2'   | 27:DA:853:G:H8     | 1.56                     | 0.69              |
| 41:DS:28:VAL:O    | 41:DS:89:ARG:HG2   | 1.91                     | 0.69              |
| 27:DA:495:G:H1'   | 45:DW:57:ASN:HD21  | 1.58                     | 0.69              |
| 1:AA:193:C:O2'    | 1:AA:194:C:H5'     | 1.92                     | 0.69              |
| 1:AA:57:G:H2'     | 1:AA:58:C:H6       | 1.56                     | 0.69              |
| 1:AA:595:G:N1     | 1:AA:641:U:H2'     | 2.08                     | 0.69              |
| 1:AA:992:U:H1'    | 1:AA:993:G:C2      | 2.28                     | 0.69              |
| 3:AC:180:ALA:HB1  | 3:AC:203:PHE:HE1   | 1.57                     | 0.69              |
| 3:AC:53:ALA:O     | 3:AC:54:ARG:HB2    | 1.91                     | 0.69              |
| 5:AE:33:VAL:HG21  | 5:AE:109:ILE:HG12  | 1.74                     | 0.69              |
| 5:AE:12:LEU:HD11  | 5:AE:14:ARG:HB3    | 1.74                     | 0.69              |
| 6:AF:19:LEU:HD23  | 6:AF:19:LEU:O      | 1.93                     | 0.69              |
| 7:AG:49:ILE:HA    | 7:AG:52:GLU:HB2    | 1.75                     | 0.69              |
| 16:AP:82:GLN:H    | 16:AP:82:GLN:CD    | 1.96                     | 0.69              |
| 20:AT:80:ARG:O    | 20:AT:84:LEU:HB2   | 1.93                     | 0.69              |
| 50:B1:67:ILE:N    | 50:B1:68:PRO:HD2   | 2.07                     | 0.69              |
| 27:BA:1406:U:H2'  | 27:BA:1407:C:C6    | 2.27                     | 0.69              |
| 27:BA:2817:G:H5'' | 27:BA:2818:G:OP2   | 1.93                     | 0.69              |
| 30:BD:11:PRO:O    | 30:BD:13:ARG:N     | 2.25                     | 0.69              |
| 36:BN:4:TYR:CB    | 43:BU:64:ARG:NH2   | 2.54                     | 0.69              |
| 44:BV:47:VAL:HB   | 44:BV:50:PRO:O     | 1.91                     | 0.69              |
| 47:BY:68:HIS:HB3  | 47:BY:71:LYS:HG3   | 1.73                     | 0.69              |
| 1:CA:1120:G:H2'   | 1:CA:1121:U:C6     | 2.28                     | 0.69              |
| 8:CH:60:ARG:HG3   | 8:CH:60:ARG:NH1    | 1.99                     | 0.69              |
| 13:CM:14:ARG:O    | 13:CM:17:VAL:HG23  | 1.93                     | 0.69              |
| 49:D0:40:GLN:NE2  | 49:D0:43:THR:HA    | 2.07                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:1695:G:H2'  | 27:DA:1695:G:N3   | 2.07                     | 0.69              |
| 32:DF:65:TRP:HE3  | 32:DF:65:TRP:O    | 1.75                     | 0.69              |
| 27:DA:2009:G:H1'  | 40:DR:107:ASP:O   | 1.93                     | 0.69              |
| 42:DT:108:ARG:HA  | 42:DT:111:ARG:NH1 | 2.07                     | 0.69              |
| 1:AA:748:C:H4'    | 1:AA:749:C:O5'    | 1.92                     | 0.69              |
| 3:AC:91:LEU:HD11  | 3:AC:101:LEU:HD12 | 1.74                     | 0.69              |
| 3:AC:150:LYS:HE2  | 3:AC:152:ILE:HD11 | 1.75                     | 0.69              |
| 8:AH:2:LEU:HD13   | 8:AH:4:ASP:H      | 1.57                     | 0.69              |
| 15:AO:37:ASN:N    | 15:AO:37:ASN:ND2  | 2.40                     | 0.69              |
| 27:BA:1438:U:O2'  | 27:BA:1439:A:H5'  | 1.93                     | 0.69              |
| 27:BA:2318:G:O2'  | 27:BA:2319:G:OP1  | 2.06                     | 0.69              |
| 27:BA:2609:U:OP1  | 27:BA:2609:U:H4'  | 1.92                     | 0.69              |
| 27:BA:330:A:HO2'  | 27:BA:331:A:H8    | 1.38                     | 0.69              |
| 27:BA:484:C:H2'   | 27:BA:485:C:H6    | 1.57                     | 0.69              |
| 27:BA:699:A:H2'   | 27:BA:700:G:O4'   | 1.92                     | 0.69              |
| 27:BA:862:G:H2'   | 27:BA:863:A:O4'   | 1.93                     | 0.69              |
| 31:BE:60:ASN:CG   | 31:BE:62:PRO:HD2  | 2.13                     | 0.69              |
| 27:BA:1256:G:O2'  | 32:BF:82:ILE:HD11 | 1.91                     | 0.69              |
| 36:BN:15:LEU:HD12 | 36:BN:136:GLU:CG  | 2.22                     | 0.69              |
| 37:BO:13:ASN:ND2  | 37:BO:96:THR:H    | 1.91                     | 0.69              |
| 37:BO:22:ILE:HG12 | 37:BO:41:ALA:CA   | 2.21                     | 0.69              |
| 37:BO:78:ARG:HB2  | 37:BO:78:ARG:NH1  | 2.06                     | 0.69              |
| 39:BQ:109:VAL:CG1 | 39:BQ:113:GLN:HB3 | 2.23                     | 0.69              |
| 41:BS:14:VAL:HG12 | 41:BS:15:ARG:N    | 2.06                     | 0.69              |
| 1:CA:134:A:H61    | 16:CP:25:ARG:HH12 | 1.40                     | 0.69              |
| 4:CD:28:SER:O     | 4:CD:30:LYS:N     | 2.26                     | 0.69              |
| 6:CF:10:LEU:HD12  | 6:CF:10:LEU:N     | 2.08                     | 0.69              |
| 13:CM:25:ILE:HD11 | 13:CM:66:LEU:CD2  | 2.15                     | 0.69              |
| 13:CM:76:ALA:HA   | 13:CM:79:LYS:HG3  | 1.75                     | 0.69              |
| 21:CU:21:TYR:O    | 21:CU:22:ARG:HB2  | 1.92                     | 0.69              |
| 27:DA:2884:U:OP2  | 54:D5:43:HIS:HE1  | 1.75                     | 0.69              |
| 55:D6:19:ARG:HG2  | 55:D6:20:ASN:N    | 2.07                     | 0.69              |
| 27:DA:126:A:OP2   | 56:D7:19:ARG:HB2  | 1.93                     | 0.69              |
| 27:DA:1431:U:O2'  | 27:DA:1432:C:H5'  | 1.91                     | 0.69              |
| 27:DA:2137:C:H2'  | 27:DA:2138:C:C6   | 2.27                     | 0.69              |
| 27:DA:244:A:H2'   | 27:DA:245:G:O4'   | 1.92                     | 0.69              |
| 27:DA:267:C:H2'   | 27:DA:268:C:H6    | 1.56                     | 0.69              |
| 27:DA:2807:G:C3'  | 27:DA:2808:U:H5'' | 2.21                     | 0.69              |
| 27:DA:481:G:H1'   | 27:DA:506:G:H21   | 1.58                     | 0.69              |
| 29:DC:58:VAL:HG21 | 29:DC:166:ASP:H   | 1.58                     | 0.69              |
| 30:DD:261:LYS:NZ  | 30:DD:263:ARG:NH1 | 2.41                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DF:64:ILE:HG23  | 32:DF:65:TRP:H     | 1.57                     | 0.69              |
| 34:DH:107:VAL:CG2  | 34:DH:152:ARG:HG2  | 2.22                     | 0.69              |
| 36:DN:112:LEU:HD12 | 36:DN:115:ARG:HB3  | 1.75                     | 0.69              |
| 41:DS:74:ALA:HB1   | 41:DS:103:GLU:CB   | 2.20                     | 0.69              |
| 1:AA:627:G:O2'     | 1:AA:628:G:H5'     | 1.92                     | 0.69              |
| 4:AD:150:GLU:N     | 4:AD:150:GLU:OE1   | 2.26                     | 0.69              |
| 11:AK:84:VAL:O     | 11:AK:85:ARG:HG2   | 1.92                     | 0.69              |
| 54:B5:11:THR:HG22  | 54:B5:12:SER:O     | 1.92                     | 0.69              |
| 27:BA:1028:A:N6    | 27:BA:1125:G:H2'   | 2.08                     | 0.69              |
| 27:BA:2189:U:C3'   | 27:BA:2190:G:H5''  | 2.22                     | 0.69              |
| 27:BA:2199:A:C8    | 27:BA:2199:A:C5'   | 2.75                     | 0.69              |
| 27:BA:2512:C:H2'   | 27:BA:2513:G:O4'   | 1.92                     | 0.69              |
| 27:BA:764:A:N7     | 30:BD:209:ALA:HB3  | 2.07                     | 0.69              |
| 32:BF:126:VAL:HG21 | 32:BF:129:PHE:CZ   | 2.28                     | 0.69              |
| 37:BO:14:THR:CG2   | 37:BO:86:ILE:HD12  | 2.13                     | 0.69              |
| 42:BT:91:ARG:HB3   | 42:BT:116:ALA:CA   | 2.16                     | 0.69              |
| 45:BW:6:ILE:HA     | 45:BW:103:ILE:O    | 1.93                     | 0.69              |
| 1:CA:1215:G:H2'    | 1:CA:1216:G:C8     | 2.28                     | 0.69              |
| 1:CA:379:C:O2'     | 1:CA:380:G:H5'     | 1.92                     | 0.69              |
| 1:CA:397:A:H2'     | 1:CA:399:G:OP2     | 1.93                     | 0.69              |
| 1:CA:643:C:H5'     | 8:CH:31:PHE:CD1    | 2.27                     | 0.69              |
| 3:CC:127:ARG:HG2   | 3:CC:127:ARG:HH11  | 1.56                     | 0.69              |
| 15:CO:82:ILE:C     | 15:CO:82:ILE:HD13  | 2.12                     | 0.69              |
| 52:D3:7:LYS:CG     | 52:D3:34:GLU:HG2   | 2.22                     | 0.69              |
| 27:DA:2794:C:O2'   | 27:DA:2795:G:H5''  | 1.92                     | 0.69              |
| 27:DA:557:U:H2'    | 27:DA:558:G:H8     | 1.57                     | 0.69              |
| 27:DA:83:G:N1      | 27:DA:102:G:O2'    | 2.25                     | 0.69              |
| 28:DB:20:C:O2'     | 28:DB:21:G:H5'     | 1.92                     | 0.69              |
| 30:DD:69:ARG:HH11  | 30:DD:130:ALA:HB2  | 1.57                     | 0.69              |
| 33:DG:61:ALA:HB2   | 33:DG:68:PRO:HD3   | 1.75                     | 0.69              |
| 36:DN:120:LEU:HD11 | 36:DN:122:VAL:HG23 | 1.74                     | 0.69              |
| 36:DN:11:PRO:HB3   | 36:DN:51:PHE:CD1   | 2.28                     | 0.69              |
| 38:DP:58:THR:O     | 38:DP:61:ARG:NE    | 2.26                     | 0.69              |
| 42:DT:129:ARG:NE   | 42:DT:131:ALA:HB3  | 2.07                     | 0.69              |
| 43:DU:92:ARG:O     | 43:DU:93:LYS:HB2   | 1.93                     | 0.69              |
| 1:AA:1061:G:C5     | 1:AA:1062:U:C5     | 2.81                     | 0.69              |
| 1:AA:194:C:H2'     | 1:AA:195:A:H5''    | 1.74                     | 0.69              |
| 2:AB:132:LYS:O     | 2:AB:135:GLN:HB2   | 1.93                     | 0.69              |
| 12:AL:124:GLU:O    | 12:AL:126:ALA:N    | 2.26                     | 0.69              |
| 13:AM:52:GLU:HG2   | 13:AM:55:ARG:HH21  | 1.58                     | 0.69              |
| 27:BA:1192:G:H2'   | 27:BA:1193:G:H5'   | 1.75                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1221:C:H5'  | 27:BA:1221:C:H6    | 1.57                     | 0.69              |
| 27:BA:330:A:O2'   | 27:BA:331:A:H8     | 1.76                     | 0.69              |
| 32:BF:3:GLU:HA    | 32:BF:24:LEU:CG    | 2.22                     | 0.69              |
| 32:BF:63:LYS:NZ   | 32:BF:67:GLN:HB2   | 2.07                     | 0.69              |
| 48:BZ:76:ASP:HB2  | 48:BZ:83:GLU:HG3   | 1.75                     | 0.69              |
| 1:CA:101:A:O2'    | 1:CA:102:G:H5'     | 1.92                     | 0.69              |
| 1:CA:1238:A:N3    | 1:CA:1238:A:H2'    | 2.08                     | 0.69              |
| 1:CA:135:C:H2'    | 1:CA:136:C:H5'     | 1.74                     | 0.69              |
| 1:CA:197:A:H4'    | 1:CA:198:G:O5'     | 1.93                     | 0.69              |
| 2:CB:107:THR:O    | 2:CB:110:GLN:HG3   | 1.93                     | 0.69              |
| 2:CB:29:ALA:O     | 2:CB:32:ILE:HG22   | 1.93                     | 0.69              |
| 10:CJ:12:ASP:OD1  | 10:CJ:14:LYS:HB2   | 1.93                     | 0.69              |
| 12:CL:5:ASN:O     | 12:CL:8:VAL:HB     | 1.93                     | 0.69              |
| 13:CM:70:LEU:HD23 | 13:CM:71:ARG:N     | 2.06                     | 0.69              |
| 56:D7:9:ARG:HB3   | 56:D7:48:LYS:HZ2   | 1.57                     | 0.69              |
| 27:DA:1452:A:N6   | 27:DA:2702:U:H1'   | 2.07                     | 0.69              |
| 27:DA:1952:A:OP1  | 37:DO:44:LYS:HE2   | 1.93                     | 0.69              |
| 27:DA:2647:U:O2'  | 27:DA:2648:C:H5'   | 1.93                     | 0.69              |
| 27:DA:649:G:H2'   | 27:DA:650:C:H6     | 1.56                     | 0.69              |
| 30:DD:35:LYS:HZ1  | 30:DD:104:TYR:H    | 1.40                     | 0.69              |
| 31:DE:1:MET:HB2   | 31:DE:83:ASP:O     | 1.91                     | 0.69              |
| 31:DE:4:ILE:CG1   | 31:DE:28:ALA:HB1   | 2.23                     | 0.69              |
| 33:DG:135:LEU:H   | 33:DG:135:LEU:HD12 | 1.58                     | 0.69              |
| 33:DG:72:ARG:HH11 | 33:DG:86:MET:HG2   | 1.58                     | 0.69              |
| 38:DP:23:PRO:HB2  | 38:DP:33:ARG:NE    | 2.08                     | 0.69              |
| 27:DA:995:C:H5'   | 43:DU:54:LYS:HD3   | 1.75                     | 0.69              |
| 1:AA:1131:G:H2'   | 1:AA:1132:C:C6     | 2.28                     | 0.69              |
| 5:AE:80:ILE:HG22  | 8:AH:104:ARG:HH12  | 1.57                     | 0.69              |
| 10:AJ:39:PRO:HB3  | 10:AJ:70:ARG:CZ    | 2.22                     | 0.69              |
| 11:AK:43:SER:HA   | 11:AK:47:VAL:HG21  | 1.74                     | 0.69              |
| 20:AT:89:ARG:CZ   | 20:AT:104:LEU:HD21 | 2.22                     | 0.69              |
| 27:BA:15:G:H2'    | 27:BA:16:G:H8      | 1.58                     | 0.69              |
| 27:BA:2202:C:H2'  | 27:BA:2203:U:O4'   | 1.91                     | 0.69              |
| 27:BA:245:G:O2'   | 27:BA:246:C:H5'    | 1.93                     | 0.69              |
| 27:BA:272(B):G:H1 | 27:BA:366:C:N4     | 1.90                     | 0.69              |
| 31:BE:16:ARG:HH11 | 31:BE:16:ARG:HG3   | 1.57                     | 0.69              |
| 31:BE:36:ARG:NH2  | 31:BE:88:GLY:CA    | 2.54                     | 0.69              |
| 32:BF:84:VAL:HG12 | 32:BF:85:GLY:N     | 2.07                     | 0.69              |
| 33:BG:56:ALA:CB   | 33:BG:153:ARG:HH21 | 2.06                     | 0.69              |
| 35:BI:133:HIS:H   | 35:BI:133:HIS:CD2  | 2.10                     | 0.69              |
| 38:BP:83:VAL:HG21 | 38:BP:105:LEU:HD12 | 1.73                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BT:42:ILE:O     | 42:BT:42:ILE:HD12  | 1.93                     | 0.69              |
| 47:BY:87:LYS:CG    | 47:BY:88:LYS:H     | 2.05                     | 0.69              |
| 1:CA:646:U:O2'     | 1:CA:647:C:H5'     | 1.92                     | 0.69              |
| 5:CE:101:ILE:H     | 5:CE:101:ILE:HD13  | 1.58                     | 0.69              |
| 20:CT:33:ILE:HD13  | 20:CT:62:LEU:HB3   | 1.75                     | 0.69              |
| 55:D6:33:LYS:CA    | 55:D6:33:LYS:HE2   | 2.16                     | 0.69              |
| 27:DA:1260:G:H2'   | 27:DA:1261:C:H6    | 1.57                     | 0.69              |
| 27:DA:1814:G:H2'   | 27:DA:1815:A:N7    | 2.08                     | 0.69              |
| 27:DA:1899:G:N2    | 27:DA:1902:C:H41   | 1.91                     | 0.69              |
| 27:DA:2110:G:H5''  | 27:DA:2111:C:OP2   | 1.93                     | 0.69              |
| 27:DA:2258:C:H6    | 27:DA:2426:A:H5'   | 1.58                     | 0.69              |
| 27:DA:271(A):A:H5' | 27:DA:271(B):C:OP2 | 1.93                     | 0.69              |
| 27:DA:707:G:H1     | 27:DA:724:U:H3     | 1.40                     | 0.69              |
| 34:DH:106:THR:CG2  | 34:DH:112:PRO:HB3  | 2.23                     | 0.69              |
| 41:DS:66:ALA:O     | 41:DS:69:VAL:HG12  | 1.93                     | 0.69              |
| 44:DV:99:ILE:HD13  | 44:DV:99:ILE:N     | 2.08                     | 0.69              |
| 45:DW:4:LYS:HA     | 45:DW:106:ILE:HG22 | 1.75                     | 0.69              |
| 46:DX:12:VAL:CG1   | 46:DX:17:ALA:HB1   | 2.23                     | 0.69              |
| 1:AA:935:A:N6      | 7:AG:3:ARG:HB2     | 2.08                     | 0.69              |
| 8:AH:60:ARG:NH1    | 8:AH:60:ARG:HG3    | 2.01                     | 0.69              |
| 38:BP:65:ARG:HH21  | 57:B8:15:LYS:HB2   | 1.54                     | 0.69              |
| 27:BA:1887:C:C2'   | 27:BA:1888:G:H5''  | 2.22                     | 0.69              |
| 27:BA:2161:C:H2'   | 27:BA:2162:G:H8    | 1.57                     | 0.69              |
| 27:BA:922:U:H2'    | 27:BA:923:C:C6     | 2.27                     | 0.69              |
| 35:BI:13:GLY:O     | 35:BI:14:ASP:HB2   | 1.92                     | 0.69              |
| 37:BO:13:ASN:ND2   | 37:BO:97:ARG:N     | 2.41                     | 0.69              |
| 37:BO:14:THR:HG21  | 37:BO:86:ILE:CD1   | 2.13                     | 0.69              |
| 48:BZ:149:LEU:CD2  | 48:BZ:170:ILE:HG13 | 2.22                     | 0.69              |
| 1:CA:1515:C:O2'    | 1:CA:1516:G:H5'    | 1.92                     | 0.69              |
| 1:CA:602:A:O2'     | 1:CA:603:U:H5'     | 1.92                     | 0.69              |
| 1:CA:628:G:H2'     | 1:CA:629:G:C8      | 2.28                     | 0.69              |
| 8:CH:4:ASP:OD1     | 8:CH:7:ALA:N       | 2.26                     | 0.69              |
| 25:CY:68:C:C3'     | 25:CY:69:C:H5''    | 2.23                     | 0.69              |
| 57:D8:61:LEU:HD13  | 57:D8:62:LEU:HG    | 1.75                     | 0.69              |
| 27:DA:1440:G:H2'   | 27:DA:1441:G:C8    | 2.28                     | 0.69              |
| 27:DA:1493:C:O2    | 27:DA:1493:C:H2'   | 1.92                     | 0.69              |
| 27:DA:2547:U:H2'   | 27:DA:2548:G:H8    | 1.57                     | 0.69              |
| 27:DA:271(E):U:H2' | 27:DA:271(F):C:C6  | 2.28                     | 0.69              |
| 27:DA:65:C:O2'     | 27:DA:66:C:H5'     | 1.93                     | 0.69              |
| 27:DA:862:G:H2'    | 27:DA:863:A:O4'    | 1.92                     | 0.69              |
| 32:DF:7:TYR:HB3    | 32:DF:16:GLY:N     | 1.99                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DH:103:LEU:HD23 | 34:DH:115:VAL:HB   | 1.74                     | 0.69              |
| 40:DR:30:THR:O     | 40:DR:30:THR:HG23  | 1.92                     | 0.69              |
| 46:DX:51:VAL:HG11  | 46:DX:81:VAL:HB    | 1.74                     | 0.69              |
| 48:DZ:38:VAL:HG21  | 48:DZ:43:PHE:HB2   | 1.74                     | 0.69              |
| 1:AA:1016:A:H2'    | 1:AA:1017:G:O4'    | 1.93                     | 0.68              |
| 3:AC:118:GLN:O     | 3:AC:122:GLU:HG3   | 1.93                     | 0.68              |
| 3:AC:189:ALA:HB3   | 3:AC:196:LEU:HB2   | 1.75                     | 0.68              |
| 4:AD:33:MET:HE2    | 4:AD:37:PRO:HA     | 1.75                     | 0.68              |
| 10:AJ:80:LYS:HE3   | 10:AJ:80:LYS:O     | 1.92                     | 0.68              |
| 12:AL:3:THR:N      | 12:AL:6:GLN:NE2    | 2.41                     | 0.68              |
| 27:BA:191:A:H2'    | 27:BA:192:C:C6     | 2.28                     | 0.68              |
| 27:BA:2712:U:H1'   | 27:BA:2712(A):A:C8 | 2.29                     | 0.68              |
| 27:BA:70:G:HO2'    | 27:BA:114:U:H5     | 1.40                     | 0.68              |
| 32:BF:134:GLY:HA2  | 32:BF:166:ALA:HB2  | 1.75                     | 0.68              |
| 43:BU:91:ASP:O     | 43:BU:92:ARG:HD3   | 1.93                     | 0.68              |
| 1:CA:1093:A:O2'    | 1:CA:1094:G:H5'    | 1.93                     | 0.68              |
| 1:CA:115:G:H4'     | 1:CA:116:A:O5'     | 1.92                     | 0.68              |
| 1:CA:767:A:H2'     | 1:CA:768:A:C8      | 2.27                     | 0.68              |
| 27:DA:2142:C:H2'   | 27:DA:2143:C:C6    | 2.29                     | 0.68              |
| 27:DA:2322:A:H2'   | 27:DA:2323:G:O4'   | 1.92                     | 0.68              |
| 27:DA:2514:U:O2'   | 27:DA:2515:C:H5'   | 1.93                     | 0.68              |
| 27:DA:2672:G:H3'   | 27:DA:2673:G:H5''  | 1.74                     | 0.68              |
| 27:DA:291:C:H2'    | 27:DA:292:C:H6     | 1.56                     | 0.68              |
| 27:DA:847:U:H2'    | 27:DA:848:G:H5''   | 1.73                     | 0.68              |
| 28:DB:15:A:H3'     | 28:DB:16:G:H5'     | 1.74                     | 0.68              |
| 28:DB:26:A:H8      | 28:DB:26:A:H5''    | 1.58                     | 0.68              |
| 37:DO:12:ASP:HA    | 37:DO:98:VAL:HA    | 1.75                     | 0.68              |
| 39:DQ:34:LEU:N     | 39:DQ:104:PHE:O    | 2.24                     | 0.68              |
| 42:DT:32:TYR:O     | 42:DT:41:ARG:O     | 2.11                     | 0.68              |
| 46:DX:55:ASN:HB2   | 46:DX:80:ILE:HD13  | 1.75                     | 0.68              |
| 48:DZ:150:HIS:HB2  | 48:DZ:167:GLU:O    | 1.93                     | 0.68              |
| 1:AA:1437:C:H42    | 1:AA:1464:G:H1     | 1.38                     | 0.68              |
| 1:AA:308:C:H2'     | 1:AA:309:G:C8      | 2.28                     | 0.68              |
| 2:AB:167:PRO:O     | 2:AB:171:ALA:N     | 2.27                     | 0.68              |
| 49:B0:25:ARG:HG2   | 49:B0:25:ARG:HH11  | 1.57                     | 0.68              |
| 27:BA:786:C:H4'    | 27:BA:1780:A:N7    | 2.09                     | 0.68              |
| 28:BB:40:U:C2      | 28:BB:43:C:H5''    | 2.28                     | 0.68              |
| 30:BD:227:ASN:C    | 30:BD:234:GLY:HA3  | 2.13                     | 0.68              |
| 32:BF:160:ASN:HD21 | 32:BF:162:LEU:CB   | 2.06                     | 0.68              |
| 32:BF:18:ARG:HG2   | 32:BF:199:TRP:CZ3  | 2.28                     | 0.68              |
| 35:BI:5:LEU:HD12   | 35:BI:5:LEU:N      | 2.08                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BI:82:ARG:HB2  | 35:BI:82:ARG:NH1   | 2.08                     | 0.68              |
| 38:BP:112:LEU:N   | 38:BP:128:HIS:HD2  | 1.87                     | 0.68              |
| 42:BT:31:SER:C    | 42:BT:32:TYR:HD2   | 1.96                     | 0.68              |
| 1:CA:1178:G:OP2   | 9:CI:97:LYS:HE3    | 1.94                     | 0.68              |
| 1:CA:1307:U:H2'   | 1:CA:1308:U:H6     | 1.58                     | 0.68              |
| 1:CA:970:C:H41    | 9:CI:126:SER:HB3   | 1.56                     | 0.68              |
| 2:CB:102:LEU:O    | 2:CB:105:PHE:HB2   | 1.93                     | 0.68              |
| 19:CS:62:ILE:O    | 19:CS:62:ILE:HG23  | 1.93                     | 0.68              |
| 23:CW:21:A:H2'    | 23:CW:22:G:O4'     | 1.93                     | 0.68              |
| 13:CM:118:ALA:HB2 | 24:CX:28:C:H4'     | 1.75                     | 0.68              |
| 57:D8:32:LEU:O    | 57:D8:33:ASN:O     | 2.11                     | 0.68              |
| 27:DA:1356:G:H2'  | 27:DA:1357:U:C6    | 2.27                     | 0.68              |
| 27:DA:1403:C:H5'' | 27:DA:1471:A:C1'   | 2.22                     | 0.68              |
| 27:DA:2238:G:H4'  | 27:DA:2239:G:N7    | 2.08                     | 0.68              |
| 27:DA:2702:U:H2'  | 27:DA:2702:U:O2    | 1.92                     | 0.68              |
| 33:DG:15:VAL:C    | 33:DG:17:PRO:HD2   | 2.14                     | 0.68              |
| 35:DI:81:VAL:HG21 | 35:DI:142:VAL:HG13 | 1.75                     | 0.68              |
| 36:DN:42:TRP:CD1  | 43:DU:63:VAL:HG11  | 2.28                     | 0.68              |
| 41:DS:92:TYR:CD1  | 41:DS:93:LYS:N     | 2.60                     | 0.68              |
| 27:DA:2012:G:H4'  | 45:DW:96:ILE:HD11  | 1.74                     | 0.68              |
| 1:AA:1225:A:OP2   | 1:AA:1226:C:H5     | 1.76                     | 0.68              |
| 1:AA:567:G:C2     | 1:AA:568:G:H1'     | 2.27                     | 0.68              |
| 1:AA:723:U:O2'    | 1:AA:724:G:H5'     | 1.92                     | 0.68              |
| 1:AA:792:A:H4'    | 1:AA:793:U:O5'     | 1.93                     | 0.68              |
| 3:AC:100:ALA:O    | 3:AC:101:LEU:HB2   | 1.93                     | 0.68              |
| 16:AP:19:ILE:HD11 | 16:AP:73:LEU:HD12  | 1.73                     | 0.68              |
| 25:AY:18:G:H4'    | 25:AY:56:G:H22     | 1.58                     | 0.68              |
| 27:BA:1835:G:N3   | 27:BA:1835:G:H2'   | 2.07                     | 0.68              |
| 27:BA:2402:C:H2'  | 27:BA:2403:C:H5'   | 1.75                     | 0.68              |
| 27:BA:275:G:O3'   | 27:BA:279:C:P      | 2.52                     | 0.68              |
| 27:BA:2853:C:H2'  | 27:BA:2854:G:C8    | 2.28                     | 0.68              |
| 27:BA:352:G:N3    | 27:BA:352:G:H2'    | 2.09                     | 0.68              |
| 27:BA:985:C:H2'   | 27:BA:986:C:C6     | 2.28                     | 0.68              |
| 30:BD:181:GLU:HA  | 30:BD:272:ALA:HB3  | 1.75                     | 0.68              |
| 30:BD:44:ASN:HB3  | 30:BD:49:ILE:HA    | 1.73                     | 0.68              |
| 36:BN:46:VAL:O    | 36:BN:47:ALA:CB    | 2.40                     | 0.68              |
| 37:BO:14:THR:HG22 | 37:BO:16:ALA:H     | 1.56                     | 0.68              |
| 41:BS:77:ALA:O    | 41:BS:79:ALA:N     | 2.27                     | 0.68              |
| 47:BY:67:LEU:CD1  | 47:BY:71:LYS:HE3   | 2.24                     | 0.68              |
| 1:CA:1460:A:H2'   | 1:CA:1461:G:O4'    | 1.93                     | 0.68              |
| 1:CA:261:U:O2     | 1:CA:263:A:C8      | 2.46                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:685:G:C2     | 1:CA:686:U:C5      | 2.81                     | 0.68              |
| 1:CA:939:G:H5''   | 7:CG:102:ARG:NH2   | 2.07                     | 0.68              |
| 5:CE:64:ARG:HE    | 5:CE:64:ARG:HA     | 1.58                     | 0.68              |
| 10:CJ:35:SER:OG   | 10:CJ:73:ASP:HB2   | 1.94                     | 0.68              |
| 11:CK:85:ARG:HG2  | 11:CK:111:ASP:O    | 1.92                     | 0.68              |
| 10:CJ:61:GLU:CD   | 14:CN:58:LYS:HE2   | 2.14                     | 0.68              |
| 24:CX:17:C:H3'    | 24:CX:17(B):U:H5'  | 1.75                     | 0.68              |
| 27:DA:857:C:P     | 49:D0:77:ARG:HH22  | 2.17                     | 0.68              |
| 51:D2:16:LEU:O    | 51:D2:20:GLU:HB3   | 1.94                     | 0.68              |
| 27:DA:1332:G:H5'  | 27:DA:1333:C:OP2   | 1.92                     | 0.68              |
| 27:DA:633:A:C2'   | 27:DA:634:C:H5'    | 2.21                     | 0.68              |
| 35:DI:10:GLU:O    | 35:DI:12:LEU:HD23  | 1.93                     | 0.68              |
| 38:DP:96:THR:O    | 38:DP:100:LEU:HD23 | 1.94                     | 0.68              |
| 38:DP:41:ARG:NE   | 38:DP:41:ARG:HA    | 2.08                     | 0.68              |
| 42:DT:129:ARG:CD  | 42:DT:131:ALA:HB3  | 2.24                     | 0.68              |
| 42:DT:28:VAL:CG2  | 42:DT:47:GLY:H     | 1.98                     | 0.68              |
| 1:AA:460:G:C6     | 1:AA:470:C:H5''    | 2.29                     | 0.68              |
| 6:AF:55:ASP:HB2   | 6:AF:86:ARG:HH22   | 1.57                     | 0.68              |
| 1:AA:568:G:O6     | 12:AL:2:PRO:HD3    | 1.93                     | 0.68              |
| 12:AL:92:GLY:O    | 12:AL:94:ARG:HG3   | 1.94                     | 0.68              |
| 52:B3:23:LEU:N    | 52:B3:23:LEU:HD12  | 2.01                     | 0.68              |
| 27:BA:1784:A:H4'  | 27:BA:1785:A:C5'   | 2.22                     | 0.68              |
| 27:BA:2296:U:H4'  | 27:BA:2297:C:OP1   | 1.93                     | 0.68              |
| 27:BA:382:G:C2'   | 27:BA:383:U:H5'    | 2.24                     | 0.68              |
| 27:BA:782:A:H5'   | 27:BA:783:A:C2     | 2.29                     | 0.68              |
| 28:BB:105:A:H2'   | 28:BB:106:G:O4'    | 1.94                     | 0.68              |
| 30:BD:134:ARG:HD3 | 30:BD:135:PHE:CE1  | 2.28                     | 0.68              |
| 30:BD:243:GLY:O   | 30:BD:244:ARG:CB   | 2.42                     | 0.68              |
| 32:BF:65:TRP:HB3  | 32:BF:66:PRO:HD3   | 1.75                     | 0.68              |
| 38:BP:97:PRO:O    | 38:BP:98:GLU:HG3   | 1.93                     | 0.68              |
| 48:BZ:111:ARG:HG2 | 48:BZ:111:ARG:HH11 | 1.58                     | 0.68              |
| 1:CA:52:G:H2'     | 1:CA:53:A:C8       | 2.26                     | 0.68              |
| 2:CB:32:ILE:CD1   | 2:CB:40:HIS:HB3    | 2.20                     | 0.68              |
| 5:CE:19:MET:SD    | 5:CE:24:ARG:HB3    | 2.33                     | 0.68              |
| 8:CH:20:TYR:HA    | 8:CH:65:TYR:HE2    | 1.58                     | 0.68              |
| 8:CH:86:ILE:HG22  | 8:CH:87:SER:N      | 2.08                     | 0.68              |
| 10:CJ:63:PHE:HB3  | 14:CN:57:ARG:O     | 1.92                     | 0.68              |
| 17:CQ:81:ARG:NH1  | 17:CQ:84:LEU:HD11  | 2.08                     | 0.68              |
| 1:CA:1494:G:C8    | 26:CZ:3:SER:HB3    | 2.28                     | 0.68              |
| 56:D7:22:MET:SD   | 56:D7:31:LEU:HD11  | 2.34                     | 0.68              |
| 27:DA:2000:G:O2'  | 27:DA:2001:A:H5'   | 1.93                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:DC:100:ILE:HD13 | 29:DC:132:GLY:HA3  | 1.75                     | 0.68              |
| 30:DD:2:ALA:O      | 30:DD:3:VAL:HB     | 1.92                     | 0.68              |
| 34:DH:137:ASP:OD1  | 34:DH:138:LYS:N    | 2.25                     | 0.68              |
| 36:DN:17:ASP:OD2   | 36:DN:56:ASN:HB3   | 1.92                     | 0.68              |
| 41:DS:52:SER:CB    | 41:DS:55:ALA:HB3   | 2.17                     | 0.68              |
| 44:DV:75:PHE:HE2   | 44:DV:82:ARG:NE    | 1.92                     | 0.68              |
| 47:DY:88:LYS:HE2   | 47:DY:93:GLY:HA3   | 1.76                     | 0.68              |
| 1:AA:1028:C:H42    | 1:AA:1034:G:N2     | 1.92                     | 0.68              |
| 1:AA:1082:G:O2'    | 1:AA:1083:U:H5'    | 1.94                     | 0.68              |
| 1:AA:658:G:OP1     | 15:AO:31:LEU:HD21  | 1.94                     | 0.68              |
| 1:AA:979:C:H3'     | 1:AA:980:C:C5'     | 2.24                     | 0.68              |
| 4:AD:22:LYS:HB2    | 4:AD:26:CYS:HB2    | 1.74                     | 0.68              |
| 7:AG:24:THR:HA     | 7:AG:27:ILE:CD1    | 2.24                     | 0.68              |
| 8:AH:86:ILE:HD11   | 8:AH:136:GLU:HB3   | 1.75                     | 0.68              |
| 15:AO:82:ILE:O     | 15:AO:82:ILE:HD13  | 1.93                     | 0.68              |
| 1:AA:1456:G:O3'    | 20:AT:39:LYS:NZ    | 2.24                     | 0.68              |
| 27:BA:1667:G:N3    | 27:BA:1991:U:C5    | 2.62                     | 0.68              |
| 27:BA:2331:G:H4'   | 49:B0:43:THR:N     | 2.05                     | 0.68              |
| 27:BA:534:U:H2'    | 27:BA:535:C:C6     | 2.29                     | 0.68              |
| 28:BB:21:G:H2'     | 28:BB:22:U:H6      | 1.58                     | 0.68              |
| 31:BE:26:ILE:O     | 31:BE:181:LEU:HD12 | 1.94                     | 0.68              |
| 34:BH:54:ARG:HG2   | 34:BH:65:HIS:HD2   | 1.58                     | 0.68              |
| 35:BI:68:LEU:HA    | 35:BI:71:ILE:HG13  | 1.75                     | 0.68              |
| 40:BR:76:VAL:CG1   | 40:BR:77:ARG:N     | 2.56                     | 0.68              |
| 41:BS:105:ALA:C    | 41:BS:107:GLU:H    | 1.96                     | 0.68              |
| 1:CA:1030:C:H2'    | 1:CA:1030(A):G:H5' | 1.76                     | 0.68              |
| 1:CA:1419:G:H2'    | 1:CA:1420:C:H6     | 1.59                     | 0.68              |
| 1:CA:445:G:H1      | 1:CA:489:C:H42     | 1.42                     | 0.68              |
| 13:CM:22:ILE:HG22  | 13:CM:25:ILE:HD13  | 1.76                     | 0.68              |
| 13:CM:81:LEU:HD22  | 13:CM:86:CYS:SG    | 2.34                     | 0.68              |
| 19:CS:15:LEU:O     | 19:CS:19:VAL:HG23  | 1.94                     | 0.68              |
| 20:CT:16:HIS:HA    | 20:CT:19:SER:HB3   | 1.75                     | 0.68              |
| 24:CX:64:G:H2'     | 24:CX:65:C:C6      | 2.27                     | 0.68              |
| 50:D1:7:ILE:HB     | 50:D1:62:VAL:HG23  | 1.75                     | 0.68              |
| 27:DA:1024:G:H3'   | 27:DA:1025:G:H5''  | 1.74                     | 0.68              |
| 27:DA:271(R):G:H2' | 27:DA:271(S):G:H8  | 1.58                     | 0.68              |
| 27:DA:2821:A:H2'   | 27:DA:2822:G:H8    | 1.58                     | 0.68              |
| 27:DA:321:G:OP2    | 32:DF:135:LYS:HD2  | 1.93                     | 0.68              |
| 27:DA:779:U:OP1    | 30:DD:49:ILE:HG22  | 1.94                     | 0.68              |
| 30:DD:72:LYS:HD2   | 30:DD:97:TYR:CD1   | 2.27                     | 0.68              |
| 35:DI:37:VAL:HG12  | 35:DI:38:LEU:N     | 2.07                     | 0.68              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 39:DQ:26:TYR:O      | 39:DQ:67:ARG:NH1   | 2.26                     | 0.68              |
| 42:DT:65:LYS:HZ2    | 42:DT:66:VAL:H     | 0.73                     | 0.68              |
| 42:DT:80:SER:CB     | 42:DT:81:PRO:HD2   | 2.23                     | 0.68              |
| 47:DY:15:VAL:HG12   | 47:DY:17:SER:H     | 1.58                     | 0.68              |
| 47:DY:27:VAL:HG12   | 47:DY:29:GLU:H     | 1.58                     | 0.68              |
| 1:AA:114:U:H2'      | 1:AA:115:G:C8      | 2.29                     | 0.68              |
| 8:AH:86:ILE:HG12    | 8:AH:135:CYS:HA    | 1.74                     | 0.68              |
| 10:AJ:46:ARG:HA     | 10:AJ:64:GLU:HB3   | 1.76                     | 0.68              |
| 51:B2:7:ARG:HH11    | 51:B2:7:ARG:HG2    | 1.57                     | 0.68              |
| 55:B6:19:ARG:O      | 55:B6:20:ASN:O     | 2.10                     | 0.68              |
| 27:BA:2670:A:OP2    | 27:BA:2670:A:H8    | 1.76                     | 0.68              |
| 27:BA:85:G:OP1      | 47:BY:9:LYS:HA     | 1.94                     | 0.68              |
| 28:BB:3:C:N4        | 28:BB:118:G:H1     | 1.86                     | 0.68              |
| 32:BF:1:MET:HG2     | 32:BF:26:ALA:HA    | 1.73                     | 0.68              |
| 2:CB:107:THR:HG23   | 2:CB:110:GLN:NE2   | 2.09                     | 0.68              |
| 1:CA:403:C:OP1      | 4:CD:136:PRO:HD2   | 1.93                     | 0.68              |
| 1:CA:1367:C:OP1     | 9:CI:114:TYR:HA    | 1.94                     | 0.68              |
| 24:CX:19:G:H5'      | 24:CX:20:U:C5      | 2.28                     | 0.68              |
| 27:DA:1142(A):A:O2' | 27:DA:1143:A:H2'   | 1.93                     | 0.68              |
| 27:DA:2256:G:N2     | 27:DA:2275:C:C4    | 2.62                     | 0.68              |
| 27:DA:363:G:H2'     | 27:DA:363(A):A:H8  | 1.59                     | 0.68              |
| 27:DA:839:U:H2'     | 27:DA:840:C:C6     | 2.29                     | 0.68              |
| 30:DD:218:ARG:CB    | 30:DD:219:PRO:HD2  | 2.22                     | 0.68              |
| 36:DN:60:ILE:CD1    | 36:DN:99:LEU:HD23  | 2.23                     | 0.68              |
| 45:DW:10:VAL:HG23   | 45:DW:101:SER:O    | 1.92                     | 0.68              |
| 1:AA:1442(A):G:H4'  | 1:AA:1442(B):A:OP2 | 1.92                     | 0.68              |
| 8:AH:77:GLU:HG2     | 8:AH:78:GLN:H      | 1.59                     | 0.68              |
| 10:AJ:84:GLN:O      | 10:AJ:85:LEU:HD23  | 1.94                     | 0.68              |
| 24:AX:64:G:H2'      | 24:AX:65:C:C6      | 2.28                     | 0.68              |
| 25:AY:3:G:H1        | 25:AY:69:C:H42     | 1.42                     | 0.68              |
| 49:B0:68:GLU:HG2    | 49:B0:80:HIS:HB2   | 1.74                     | 0.68              |
| 27:BA:1615:C:H2'    | 27:BA:1617:C:C5    | 2.28                     | 0.68              |
| 27:BA:1935:G:H1'    | 27:BA:1964:G:N2    | 2.08                     | 0.68              |
| 27:BA:2758:A:C2'    | 27:BA:2759:G:H5'   | 2.24                     | 0.68              |
| 27:BA:436:C:H2'     | 27:BA:437:G:C8     | 2.29                     | 0.68              |
| 27:BA:857:C:H5'     | 49:B0:77:ARG:NH2   | 2.03                     | 0.68              |
| 31:BE:117:MET:O     | 31:BE:118:LYS:HB2  | 1.92                     | 0.68              |
| 27:BA:320:A:OP2     | 32:BF:137:LYS:HD2  | 1.94                     | 0.68              |
| 32:BF:18:ARG:HG2    | 32:BF:199:TRP:HZ3  | 1.59                     | 0.68              |
| 34:BH:85:LYS:HZ3    | 34:BH:133:VAL:HG21 | 1.55                     | 0.68              |
| 40:BR:10:LEU:HD22   | 40:BR:17:ARG:NH1   | 2.08                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BT:81:PRO:O     | 42:BT:82:LEU:HG    | 1.94                     | 0.68              |
| 43:BU:8:VAL:HG11   | 43:BU:12:ARG:HE    | 1.58                     | 0.68              |
| 1:CA:841:U:O2'     | 1:CA:848:C:H5'     | 1.94                     | 0.68              |
| 2:CB:219:VAL:HA    | 2:CB:222:ILE:HD12  | 1.74                     | 0.68              |
| 16:CP:56:ALA:O     | 16:CP:60:LEU:HG    | 1.92                     | 0.68              |
| 12:CL:5:ASN:HD22   | 17:CQ:34:LYS:NZ    | 1.91                     | 0.68              |
| 52:D3:7:LYS:CB     | 52:D3:34:GLU:HG2   | 2.24                     | 0.68              |
| 53:D4:62:CYS:SG    | 53:D4:64:LYS:HB2   | 2.33                     | 0.68              |
| 57:D8:61:LEU:CD1   | 57:D8:62:LEU:H     | 2.05                     | 0.68              |
| 27:DA:324:A:C2     | 27:DA:325:G:H1'    | 2.28                     | 0.68              |
| 27:DA:307:G:H21    | 27:DA:330:A:H62    | 1.40                     | 0.68              |
| 30:DD:11:PRO:O     | 30:DD:13:ARG:N     | 2.27                     | 0.68              |
| 32:DF:41:LEU:HD11  | 32:DF:184:TYR:CE1  | 2.29                     | 0.68              |
| 32:DF:89:VAL:HG12  | 32:DF:90:PHE:N     | 2.08                     | 0.68              |
| 33:DG:76:SER:CA    | 33:DG:83:ARG:HB2   | 2.24                     | 0.68              |
| 33:DG:44:GLY:N     | 33:DG:88:ILE:HG12  | 2.07                     | 0.68              |
| 38:DP:113:LYS:HA   | 38:DP:129:ALA:O    | 1.93                     | 0.68              |
| 38:DP:46:LYS:NZ    | 38:DP:51:PHE:CE2   | 2.62                     | 0.68              |
| 45:DW:4:LYS:HG2    | 45:DW:106:ILE:HG22 | 1.75                     | 0.68              |
| 1:AA:1066:C:H2'    | 1:AA:1067:A:C8     | 2.29                     | 0.68              |
| 1:AA:1202:G:C2     | 14:AN:42:ILE:HG21  | 2.29                     | 0.68              |
| 1:AA:1128:C:H5'    | 9:AI:16:ARG:HH12   | 1.58                     | 0.68              |
| 13:AM:5:ALA:HB2    | 13:AM:66:LEU:HD22  | 1.76                     | 0.68              |
| 16:AP:23:ASP:O     | 16:AP:25:ARG:N     | 2.27                     | 0.68              |
| 18:AR:31:LEU:HD11  | 18:AR:62:GLU:HG2   | 1.75                     | 0.68              |
| 51:B2:4:SER:HA     | 51:B2:7:ARG:NH1    | 2.09                     | 0.68              |
| 27:BA:2562:U:H2'   | 27:BA:2563:U:H5'   | 1.74                     | 0.68              |
| 27:BA:719:C:O2'    | 27:BA:720:C:H5'    | 1.94                     | 0.68              |
| 27:BA:90:U:H1'     | 27:BA:92:A:H8      | 1.57                     | 0.68              |
| 28:BB:35:U:H2'     | 28:BB:36:C:C6      | 2.28                     | 0.68              |
| 35:BI:131:LYS:HG3  | 35:BI:132:PRO:HD2  | 1.74                     | 0.68              |
| 39:BQ:109:VAL:HG13 | 39:BQ:113:GLN:OE1  | 1.94                     | 0.68              |
| 41:BS:25:ARG:O     | 41:BS:39:ILE:HA    | 1.92                     | 0.68              |
| 48:BZ:156:LEU:HB3  | 48:BZ:160:VAL:HG12 | 1.75                     | 0.68              |
| 1:CA:1251:A:H2'    | 1:CA:1252:A:H8     | 1.56                     | 0.68              |
| 1:CA:164:U:H2'     | 1:CA:165:C:C6      | 2.29                     | 0.68              |
| 2:CB:80:ILE:CD1    | 2:CB:212:GLN:HA    | 2.23                     | 0.68              |
| 7:CG:75:VAL:HG12   | 7:CG:88:PRO:HB3    | 1.74                     | 0.68              |
| 11:CK:21:ILE:CD1   | 11:CK:82:VAL:HG13  | 2.24                     | 0.68              |
| 11:CK:67:ASP:O     | 11:CK:70:LYS:HB3   | 1.94                     | 0.68              |
| 13:CM:22:ILE:HB    | 13:CM:25:ILE:HB    | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:71:A:H5''   | 27:DA:73:A:N7     | 2.09                     | 0.68              |
| 42:DT:31:SER:HB2  | 42:DT:32:TYR:CE2  | 2.29                     | 0.68              |
| 1:AA:1171:G:H2'   | 1:AA:1172:C:H6    | 1.59                     | 0.68              |
| 3:AC:150:LYS:HE3  | 3:AC:167:TRP:HE1  | 1.58                     | 0.68              |
| 7:AG:105:VAL:O    | 7:AG:108:ALA:HB3  | 1.94                     | 0.68              |
| 9:AI:4:TYR:HD1    | 9:AI:4:TYR:N      | 1.92                     | 0.68              |
| 1:AA:523:A:C2     | 12:AL:88:LYS:HB3  | 2.29                     | 0.68              |
| 57:B8:11:LYS:HG3  | 57:B8:64:TYR:OH   | 1.94                     | 0.68              |
| 27:BA:2111:C:H4'  | 27:BA:2112:G:OP1  | 1.94                     | 0.68              |
| 27:BA:623:G:H2'   | 27:BA:624:C:C6    | 2.28                     | 0.68              |
| 32:BF:89:VAL:HG12 | 32:BF:90:PHE:N    | 2.05                     | 0.68              |
| 36:BN:51:PHE:CE1  | 36:BN:119:ARG:HD3 | 2.29                     | 0.68              |
| 47:BY:49:VAL:O    | 47:BY:53:PRO:HG3  | 1.93                     | 0.68              |
| 47:BY:84:ARG:HB2  | 47:BY:95:LYS:O    | 1.92                     | 0.68              |
| 2:CB:161:ALA:HB1  | 2:CB:185:ILE:HD12 | 1.75                     | 0.68              |
| 7:CG:137:LYS:O    | 7:CG:141:VAL:HG23 | 1.93                     | 0.68              |
| 20:CT:30:LYS:NZ   | 20:CT:80:ARG:NH2  | 2.42                     | 0.68              |
| 55:D6:16:CYS:SG   | 55:D6:48:VAL:HG22 | 2.34                     | 0.68              |
| 57:D8:38:GLY:O    | 57:D8:42:ARG:HB2  | 1.93                     | 0.68              |
| 27:DA:197:A:H5'   | 27:DA:197:A:C8    | 2.28                     | 0.68              |
| 27:DA:541:C:H2'   | 27:DA:542:C:C5    | 2.28                     | 0.68              |
| 27:DA:548:A:O2'   | 27:DA:549:G:OP1   | 2.10                     | 0.68              |
| 28:DB:15:A:H5'    | 28:DB:16:G:C8     | 2.29                     | 0.68              |
| 38:DP:13:ASN:C    | 38:DP:13:ASN:ND2  | 2.43                     | 0.68              |
| 42:DT:109:GLU:HA  | 42:DT:112:ARG:HD3 | 1.76                     | 0.68              |
| 42:DT:13:ARG:NE   | 42:DT:13:ARG:HA   | 2.08                     | 0.68              |
| 44:DV:62:LEU:N    | 44:DV:62:LEU:HD22 | 2.08                     | 0.68              |
| 1:AA:736:C:H5''   | 18:AR:72:ARG:NH2  | 2.09                     | 0.68              |
| 4:AD:170:VAL:CG1  | 4:AD:171:GLY:N    | 2.57                     | 0.68              |
| 4:AD:57:ARG:HD3   | 4:AD:205:GLU:HB2  | 1.76                     | 0.68              |
| 17:AQ:58:GLU:C    | 17:AQ:59:ILE:HD13 | 2.14                     | 0.68              |
| 27:BA:1274:A:H1'  | 27:BA:1297:C:H4'  | 1.74                     | 0.68              |
| 27:BA:1577:C:H2'  | 27:BA:1578:U:H6   | 1.58                     | 0.68              |
| 27:BA:1615:C:H2'  | 27:BA:1617:C:H5   | 1.59                     | 0.68              |
| 27:BA:185:U:H2'   | 27:BA:186:G:H8    | 1.57                     | 0.68              |
| 27:BA:2299:G:N1   | 27:BA:2318:G:H8   | 1.90                     | 0.68              |
| 27:BA:2563:U:O2   | 27:BA:2565:A:C8   | 2.40                     | 0.68              |
| 27:BA:2790:A:H2'  | 27:BA:2790:A:N3   | 2.08                     | 0.68              |
| 30:BD:231:HIS:CD2 | 30:BD:249:PRO:HG3 | 2.28                     | 0.68              |
| 31:BE:186:GLY:O   | 31:BE:188:VAL:N   | 2.27                     | 0.68              |
| 38:BP:85:LEU:HD23 | 38:BP:85:LEU:H    | 1.59                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:200:G:H2'    | 1:CA:201:C:C6     | 2.29                     | 0.68              |
| 1:CA:93:G:O2'     | 1:CA:96:U:H5'     | 1.94                     | 0.68              |
| 7:CG:84:ASN:HD22  | 7:CG:84:ASN:H     | 1.38                     | 0.68              |
| 8:CH:28:ALA:HA    | 8:CH:59:LEU:HD11  | 1.76                     | 0.68              |
| 8:CH:48:TYR:CD1   | 8:CH:49:GLU:N     | 2.61                     | 0.68              |
| 55:D6:40:CYS:HB2  | 55:D6:46:HIS:HB3  | 1.76                     | 0.68              |
| 27:DA:1009:A:H5'  | 27:DA:1009:A:H8   | 1.58                     | 0.68              |
| 27:DA:1352:U:H3   | 27:DA:1378:A:H62  | 1.41                     | 0.68              |
| 27:DA:2086:U:H2'  | 27:DA:2087:G:C8   | 2.29                     | 0.68              |
| 27:DA:2466:C:H2'  | 27:DA:2467:C:H5'  | 1.76                     | 0.68              |
| 27:DA:2653:U:H2'  | 27:DA:2654:A:N7   | 2.09                     | 0.68              |
| 27:DA:364:C:O2    | 27:DA:364:C:H2'   | 1.93                     | 0.68              |
| 27:DA:437:G:O2'   | 27:DA:438:G:H5'   | 1.94                     | 0.68              |
| 31:DE:25:VAL:O    | 31:DE:26:ILE:HD13 | 1.93                     | 0.68              |
| 32:DF:18:ARG:HH21 | 32:DF:20:LEU:HD13 | 1.59                     | 0.68              |
| 32:DF:99:TYR:CD2  | 32:DF:99:TYR:O    | 2.47                     | 0.68              |
| 38:DP:115:LEU:HA  | 38:DP:134:ALA:CB  | 2.24                     | 0.68              |
| 38:DP:48:PRO:HG2  | 38:DP:49:ARG:N    | 1.99                     | 0.68              |
| 4:AD:59:ARG:HH21  | 4:AD:66:ARG:HH22  | 1.41                     | 0.67              |
| 1:AA:939:G:H5''   | 7:AG:102:ARG:HH12 | 1.59                     | 0.67              |
| 1:AA:640:A:C2     | 8:AH:115:SER:HB3  | 2.29                     | 0.67              |
| 9:AI:69:GLY:O     | 9:AI:73:GLN:HG3   | 1.93                     | 0.67              |
| 25:AY:12:C:H2'    | 25:AY:13:A:O4'    | 1.94                     | 0.67              |
| 49:B0:38:VAL:HG12 | 49:B0:40:GLN:HG2  | 1.74                     | 0.67              |
| 49:B0:43:THR:HG23 | 49:B0:43:THR:O    | 1.94                     | 0.67              |
| 28:BB:83:G:H4'    | 52:B3:52:HIS:CD2  | 2.28                     | 0.67              |
| 27:BA:1771:C:H5'' | 27:BA:1772:G:OP2  | 1.93                     | 0.67              |
| 27:BA:2282:G:H5'' | 27:BA:2283:C:O4'  | 1.93                     | 0.67              |
| 27:BA:610:G:H2'   | 27:BA:611:C:C6    | 2.29                     | 0.67              |
| 27:BA:673:C:H6    | 27:BA:673:C:H5''  | 1.59                     | 0.67              |
| 31:BE:69:LYS:NZ   | 31:BE:89:ASP:HA   | 2.08                     | 0.67              |
| 35:BI:64:GLU:OE1  | 35:BI:64:GLU:HA   | 1.94                     | 0.67              |
| 37:BO:103:ALA:HB1 | 37:BO:105:GLU:OE1 | 1.93                     | 0.67              |
| 27:BA:1952:A:H5'  | 37:BO:42:SER:OG   | 1.94                     | 0.67              |
| 44:BV:47:VAL:HG12 | 44:BV:52:VAL:HG12 | 1.75                     | 0.67              |
| 47:BY:42:VAL:HB   | 47:BY:65:ALA:HB3  | 1.75                     | 0.67              |
| 1:CA:1041:A:H2'   | 1:CA:1042:G:C8    | 2.28                     | 0.67              |
| 1:CA:1307:U:H2'   | 1:CA:1308:U:C6    | 2.29                     | 0.67              |
| 1:CA:376:G:O2'    | 1:CA:377:G:H5'    | 1.94                     | 0.67              |
| 1:CA:389:A:H2'    | 1:CA:390:C:O4'    | 1.94                     | 0.67              |
| 4:CD:165:MET:O    | 4:CD:166:LYS:C    | 2.32                     | 0.67              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:CF:33:TYR:CD2    | 6:CF:71:ARG:HD2   | 2.25                     | 0.67              |
| 7:CG:14:PRO:HB3    | 7:CG:19:GLY:C     | 2.15                     | 0.67              |
| 10:CJ:94:VAL:HG12  | 10:CJ:95:GLU:N    | 2.09                     | 0.67              |
| 12:CL:73:ASN:HD21  | 12:CL:105:ALA:HB2 | 1.59                     | 0.67              |
| 13:CM:23:TYR:CE1   | 13:CM:71:ARG:HB2  | 2.28                     | 0.67              |
| 13:CM:67:GLU:O     | 13:CM:69:GLU:N    | 2.27                     | 0.67              |
| 23:CW:37:U:H2'     | 23:CW:38:U:O4'    | 1.94                     | 0.67              |
| 27:DA:1033:U:H5''  | 27:DA:1034:G:OP2  | 1.95                     | 0.67              |
| 27:DA:1401:G:H2'   | 27:DA:1402:C:C6   | 2.29                     | 0.67              |
| 27:DA:1775:U:H2'   | 27:DA:1776:G:C5'  | 2.21                     | 0.67              |
| 27:DA:908:C:O2'    | 27:DA:909:A:H5'   | 1.94                     | 0.67              |
| 33:DG:68:PRO:HB2   | 33:DG:90:LEU:HD22 | 1.76                     | 0.67              |
| 37:DO:23:ARG:HD2   | 37:DO:24:VAL:H    | 1.59                     | 0.67              |
| 38:DP:13:ASN:HD22  | 38:DP:14:LYS:N    | 1.91                     | 0.67              |
| 39:DQ:79:LEU:HD22  | 39:DQ:80:GLU:N    | 2.09                     | 0.67              |
| 42:DT:14:TYR:CD1   | 42:DT:14:TYR:N    | 2.62                     | 0.67              |
| 47:DY:26:LYS:HG2   | 47:DY:27:VAL:H    | 1.59                     | 0.67              |
| 1:AA:434:U:H2'     | 1:AA:435:C:O4'    | 1.94                     | 0.67              |
| 1:AA:859:A:O2'     | 1:AA:860:A:H5'    | 1.94                     | 0.67              |
| 8:AH:39:LEU:HB2    | 8:AH:45:ILE:HD11  | 1.76                     | 0.67              |
| 10:AJ:30:SER:OG    | 10:AJ:81:THR:HG23 | 1.95                     | 0.67              |
| 12:AL:68:PRO:HG3   | 12:AL:96:HIS:HD2  | 1.59                     | 0.67              |
| 12:AL:68:PRO:O     | 12:AL:99:ARG:HD2  | 1.95                     | 0.67              |
| 49:B0:56:ASP:O     | 49:B0:57:PHE:HB2  | 1.94                     | 0.67              |
| 55:B6:11:LEU:O     | 55:B6:24:GLU:N    | 2.27                     | 0.67              |
| 27:BA:1677:A:H2'   | 27:BA:1678:G:C8   | 2.28                     | 0.67              |
| 27:BA:2693:A:H2'   | 27:BA:2694:G:H5'  | 1.76                     | 0.67              |
| 27:BA:558:G:O2'    | 27:BA:559:G:H5'   | 1.94                     | 0.67              |
| 32:BF:164:ARG:HG3  | 32:BF:175:THR:OG1 | 1.94                     | 0.67              |
| 27:BA:1190:G:H5'   | 38:BP:35:HIS:H    | 1.58                     | 0.67              |
| 38:BP:61:ARG:H     | 38:BP:61:ARG:HD2  | 1.60                     | 0.67              |
| 41:BS:19:LYS:O     | 41:BS:20:ARG:HD3  | 1.94                     | 0.67              |
| 1:CA:1148:U:H2'    | 1:CA:1149:C:O4'   | 1.94                     | 0.67              |
| 1:CA:1363(A):A:C1' | 1:CA:1365:G:N7    | 2.47                     | 0.67              |
| 1:CA:1406:U:H2'    | 1:CA:1407:C:C6    | 2.29                     | 0.67              |
| 1:CA:142:G:H1      | 1:CA:221:C:H42    | 1.38                     | 0.67              |
| 1:CA:382:A:H2'     | 1:CA:383:A:C8     | 2.29                     | 0.67              |
| 4:CD:162:LEU:O     | 4:CD:165:MET:HB2  | 1.94                     | 0.67              |
| 10:CJ:35:SER:O     | 10:CJ:36:GLY:O    | 2.12                     | 0.67              |
| 24:CX:34:C:O2      | 24:CX:34:C:H2'    | 1.94                     | 0.67              |
| 57:D8:43:GLN:O     | 57:D8:44:LYS:HD2  | 1.94                     | 0.67              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 27:DA:1142(A):A:H8 | 27:DA:1142(A):A:H5' | 1.58                     | 0.67              |
| 27:DA:1446:C:H42   | 27:DA:1465:G:H1     | 1.42                     | 0.67              |
| 27:DA:1457:A:HO2'  | 27:DA:1459:G:H8     | 1.40                     | 0.67              |
| 27:DA:1625:C:C2'   | 27:DA:1626:G:H5'    | 2.25                     | 0.67              |
| 27:DA:83:G:O2'     | 27:DA:84:A:H8       | 1.77                     | 0.67              |
| 30:DD:53:PHE:C     | 30:DD:218:ARG:HG3   | 2.15                     | 0.67              |
| 38:DP:94:GLU:HG3   | 38:DP:124:LYS:O     | 1.95                     | 0.67              |
| 42:DT:42:ILE:N     | 42:DT:42:ILE:HD12   | 2.00                     | 0.67              |
| 48:DZ:157:PRO:HG2  | 48:DZ:160:VAL:CG2   | 2.16                     | 0.67              |
| 5:AE:128:PRO:O     | 5:AE:129:ILE:O      | 2.13                     | 0.67              |
| 9:AI:106:ALA:O     | 9:AI:108:VAL:HG22   | 1.94                     | 0.67              |
| 23:AW:4:G:H2'      | 23:AW:5:G:C4'       | 2.25                     | 0.67              |
| 55:B6:13:CYS:O     | 55:B6:21:TYR:HA     | 1.93                     | 0.67              |
| 27:BA:1450:G:O2'   | 27:BA:1450(A):C:H5' | 1.93                     | 0.67              |
| 27:BA:1797:C:H4'   | 30:BD:257:LEU:O     | 1.94                     | 0.67              |
| 27:BA:2523:G:H5'   | 27:BA:2523:G:H8     | 1.59                     | 0.67              |
| 27:BA:753:C:C2'    | 27:BA:754:C:H5'     | 2.24                     | 0.67              |
| 41:BS:17:ARG:HA    | 41:BS:20:ARG:NH1    | 2.10                     | 0.67              |
| 1:CA:556:C:H2'     | 1:CA:557:G:H8       | 1.58                     | 0.67              |
| 1:CA:935:A:C2      | 1:CA:1383:C:N4      | 2.62                     | 0.67              |
| 1:CA:978:A:C8      | 1:CA:978:A:H5''     | 2.29                     | 0.67              |
| 2:CB:121:LEU:O     | 2:CB:121:LEU:HD23   | 1.95                     | 0.67              |
| 2:CB:69:LEU:HD22   | 2:CB:91:PRO:CB      | 2.17                     | 0.67              |
| 3:CC:3:ASN:O       | 3:CC:4:LYS:HB2      | 1.93                     | 0.67              |
| 5:CE:40:ARG:HB3    | 5:CE:66:MET:CE      | 2.24                     | 0.67              |
| 10:CJ:39:PRO:HB3   | 10:CJ:70:ARG:NE     | 2.09                     | 0.67              |
| 55:D6:10:LEU:H     | 55:D6:10:LEU:CD2    | 2.07                     | 0.67              |
| 57:D8:14:VAL:HG23  | 57:D8:23:VAL:O      | 1.94                     | 0.67              |
| 27:DA:2262:U:H2'   | 27:DA:2263:C:H6     | 1.59                     | 0.67              |
| 27:DA:271(A):A:H8  | 27:DA:271(B):C:C6   | 2.12                     | 0.67              |
| 33:DG:106:LEU:HD12 | 33:DG:110:ALA:HB3   | 1.74                     | 0.67              |
| 33:DG:38:VAL:HG22  | 33:DG:93:THR:HG23   | 1.76                     | 0.67              |
| 34:DH:17:VAL:O     | 34:DH:45:VAL:HG22   | 1.93                     | 0.67              |
| 38:DP:102:ARG:HB3  | 38:DP:102:ARG:CZ    | 2.23                     | 0.67              |
| 38:DP:7:ARG:H      | 38:DP:8:PRO:HD2     | 1.60                     | 0.67              |
| 40:DR:48:VAL:O     | 40:DR:51:LEU:HD12   | 1.95                     | 0.67              |
| 2:AB:77:ALA:O      | 2:AB:81:VAL:HG23    | 1.95                     | 0.67              |
| 9:AI:116:LYS:HD3   | 9:AI:122:ALA:HB2    | 1.75                     | 0.67              |
| 16:AP:48:TRP:CE3   | 16:AP:49:LEU:HB2    | 2.30                     | 0.67              |
| 51:B2:13:ALA:HA    | 51:B2:16:LEU:HD21   | 1.76                     | 0.67              |
| 27:BA:1210:A:H5'   | 27:BA:1212:G:C5'    | 2.22                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1667:G:N3    | 27:BA:1991:U:H5    | 1.92                     | 0.67              |
| 27:BA:1786:A:C2    | 27:BA:2606:C:H1'   | 2.29                     | 0.67              |
| 27:BA:2146:C:H4'   | 27:BA:2147:G:C8    | 2.30                     | 0.67              |
| 30:BD:210:GLY:O    | 30:BD:211:ARG:CB   | 2.42                     | 0.67              |
| 31:BE:170:LEU:HD23 | 31:BE:184:VAL:HG11 | 1.74                     | 0.67              |
| 35:BI:40:THR:O     | 35:BI:44:LEU:HB2   | 1.94                     | 0.67              |
| 44:BV:41:GLY:HA3   | 44:BV:45:THR:HG1   | 1.59                     | 0.67              |
| 47:BY:28:LYS:CB    | 47:BY:37:VAL:HB    | 2.24                     | 0.67              |
| 1:CA:1411:C:O2'    | 1:CA:1412:C:H5'    | 1.94                     | 0.67              |
| 1:CA:422:C:H1'     | 1:CA:423:G:N2      | 2.09                     | 0.67              |
| 2:CB:17:PHE:HB2    | 2:CB:42:ILE:CG2    | 2.25                     | 0.67              |
| 2:CB:92:TYR:O      | 2:CB:93:VAL:HG13   | 1.94                     | 0.67              |
| 5:CE:12:LEU:HD22   | 5:CE:13:ILE:H      | 1.60                     | 0.67              |
| 8:CH:104:ARG:O     | 8:CH:105:ARG:C     | 2.33                     | 0.67              |
| 9:CI:38:GLN:O      | 9:CI:40:LEU:HD23   | 1.95                     | 0.67              |
| 46:DX:60:ARG:HH22  | 56:D7:47:ARG:CZ    | 2.07                     | 0.67              |
| 27:DA:1309:G:O2'   | 27:DA:1310:G:H5'   | 1.94                     | 0.67              |
| 27:DA:1440:G:H2'   | 27:DA:1441:G:H8    | 1.58                     | 0.67              |
| 27:DA:1962:C:H4'   | 27:DA:1963:U:OP1   | 1.93                     | 0.67              |
| 27:DA:2113:U:O2'   | 27:DA:2114:A:C8    | 2.43                     | 0.67              |
| 27:DA:2626:C:H2'   | 27:DA:2627:G:C8    | 2.29                     | 0.67              |
| 31:DE:119:ARG:HD2  | 31:DE:120:TRP:CD1  | 2.29                     | 0.67              |
| 32:DF:110:LEU:O    | 32:DF:114:VAL:HG23 | 1.94                     | 0.67              |
| 35:DI:75:LEU:HD21  | 35:DI:105:HIS:HE1  | 1.57                     | 0.67              |
| 37:DO:52:VAL:C     | 37:DO:53:LYS:HD2   | 2.14                     | 0.67              |
| 37:DO:7:TYR:CE1    | 37:DO:20:MET:HE3   | 2.30                     | 0.67              |
| 40:DR:87:TYR:OH    | 40:DR:116:LEU:HB3  | 1.94                     | 0.67              |
| 40:DR:14:SER:C     | 40:DR:16:HIS:H     | 1.96                     | 0.67              |
| 46:DX:4:ALA:O      | 46:DX:7:VAL:HG23   | 1.94                     | 0.67              |
| 1:AA:1478:C:O2'    | 1:AA:1479:C:H5'    | 1.95                     | 0.67              |
| 1:AA:714:G:H21     | 1:AA:777:A:H1'     | 1.60                     | 0.67              |
| 2:AB:114:ARG:HH12  | 2:AB:118:LEU:HD21  | 1.59                     | 0.67              |
| 2:AB:178:ARG:HH12  | 2:AB:196:LEU:HB2   | 1.59                     | 0.67              |
| 3:AC:35:GLU:O      | 3:AC:39:ILE:HG13   | 1.94                     | 0.67              |
| 4:AD:3:ARG:HB3     | 4:AD:118:ARG:HH11  | 1.60                     | 0.67              |
| 5:AE:75:THR:OG1    | 5:AE:76:ILE:N      | 2.20                     | 0.67              |
| 12:AL:63:VAL:HG21  | 12:AL:95:TYR:CE1   | 2.30                     | 0.67              |
| 1:AA:267:C:OP2     | 17:AQ:67:LYS:HD2   | 1.95                     | 0.67              |
| 27:BA:1244:G:H4'   | 38:BP:11:GLY:HA2   | 1.77                     | 0.67              |
| 27:BA:1722:A:C6    | 27:BA:1740:G:C8    | 2.83                     | 0.67              |
| 27:BA:1835:G:H5'   | 27:BA:1836:C:OP2   | 1.95                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2103:C:C3'   | 27:BA:2104:G:H5''  | 2.25                     | 0.67              |
| 27:BA:2175:C:H1'   | 29:BC:215:THR:H    | 1.58                     | 0.67              |
| 27:BA:529:A:H5''   | 27:BA:530:G:OP1    | 1.95                     | 0.67              |
| 27:BA:645:C:H2'    | 27:BA:645:C:O2     | 1.93                     | 0.67              |
| 27:BA:670:A:H4'    | 27:BA:671:C:O5'    | 1.93                     | 0.67              |
| 35:BI:109:ILE:HG22 | 35:BI:111:PRO:HD3  | 1.77                     | 0.67              |
| 40:BR:18:LEU:HD11  | 40:BR:22:ARG:CZ    | 2.24                     | 0.67              |
| 42:BT:24:PRO:HA    | 42:BT:49:VAL:HG13  | 1.75                     | 0.67              |
| 42:BT:53:ARG:HD3   | 42:BT:60:THR:OG1   | 1.95                     | 0.67              |
| 42:BT:65:LYS:HZ2   | 42:BT:66:VAL:N     | 1.92                     | 0.67              |
| 43:BU:104:GLN:HE21 | 43:BU:105:VAL:N    | 1.93                     | 0.67              |
| 43:BU:88:ILE:CG2   | 44:BV:47:VAL:HG23  | 2.24                     | 0.67              |
| 48:BZ:142:GLY:C    | 48:BZ:143:LEU:HD22 | 2.14                     | 0.67              |
| 1:CA:959:A:N1      | 1:CA:1222:G:H5'    | 2.10                     | 0.67              |
| 1:CA:1468:A:H2'    | 1:CA:1469:G:O4'    | 1.95                     | 0.67              |
| 1:CA:1504:G:H4'    | 1:CA:1505:G:C5'    | 2.24                     | 0.67              |
| 1:CA:571:U:H5''    | 1:CA:819:A:C2      | 2.30                     | 0.67              |
| 3:CC:77:ILE:O      | 3:CC:83:ARG:HB3    | 1.94                     | 0.67              |
| 27:DA:2021:C:O2'   | 27:DA:2022:U:OP1   | 2.13                     | 0.67              |
| 27:DA:736:C:O2'    | 27:DA:737:C:H5'    | 1.95                     | 0.67              |
| 30:DD:133:LEU:HD13 | 30:DD:175:LEU:HD21 | 1.75                     | 0.67              |
| 33:DG:26:GLN:HB2   | 33:DG:30:GLU:OE1   | 1.94                     | 0.67              |
| 35:DI:11:ASN:O     | 35:DI:12:LEU:HB3   | 1.93                     | 0.67              |
| 35:DI:88:ILE:CD1   | 35:DI:123:LEU:HG   | 2.24                     | 0.67              |
| 38:DP:21:ARG:CD    | 38:DP:29:LYS:HE3   | 2.24                     | 0.67              |
| 38:DP:9:ASN:HD22   | 38:DP:9:ASN:N      | 1.93                     | 0.67              |
| 27:DA:560:C:C5'    | 43:DU:52:ARG:HH22  | 2.08                     | 0.67              |
| 36:DN:2:LYS:HZ3    | 44:DV:13:ARG:H     | 1.41                     | 0.67              |
| 47:DY:35:TYR:CE2   | 47:DY:69:ALA:HB3   | 2.29                     | 0.67              |
| 47:DY:76:CYS:HG    | 47:DY:77:PRO:HD2   | 1.60                     | 0.67              |
| 48:DZ:73:VAL:HG13  | 48:DZ:85:VAL:HG12  | 1.75                     | 0.67              |
| 1:AA:1457:G:O2'    | 1:AA:1458:G:H5'    | 1.94                     | 0.67              |
| 1:AA:637:G:O2'     | 1:AA:638:G:H5'     | 1.94                     | 0.67              |
| 14:AN:23:ARG:NH1   | 14:AN:30:ALA:HB2   | 2.08                     | 0.67              |
| 27:BA:1204:A:H61   | 27:BA:1240:U:H2'   | 1.59                     | 0.67              |
| 27:BA:1640:C:O2    | 27:BA:1640:C:H2'   | 1.94                     | 0.67              |
| 27:BA:2122:U:H2'   | 27:BA:2123:G:C8    | 2.29                     | 0.67              |
| 27:BA:2357:U:C2'   | 27:BA:2358:G:H5''  | 2.25                     | 0.67              |
| 27:BA:2415:G:H4'   | 38:BP:66:GLY:CA    | 2.24                     | 0.67              |
| 27:BA:2510:C:H2'   | 27:BA:2511:U:H6    | 1.60                     | 0.67              |
| 27:BA:686:G:H2'    | 27:BA:788:A:C2     | 2.29                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BE:14:ILE:HG13  | 31:BE:15:PHE:N     | 2.08                     | 0.67              |
| 31:BE:33:VAL:HG13  | 31:BE:69:LYS:CE    | 2.24                     | 0.67              |
| 31:BE:68:ALA:O     | 31:BE:70:ALA:N     | 2.28                     | 0.67              |
| 33:BG:36:LYS:HD3   | 33:BG:95:ARG:NH1   | 2.09                     | 0.67              |
| 34:BH:89:ILE:O     | 34:BH:90:LYS:O     | 2.13                     | 0.67              |
| 38:BP:85:LEU:CD2   | 38:BP:85:LEU:H     | 2.07                     | 0.67              |
| 41:BS:59:LYS:NZ    | 41:BS:68:GLN:HE22  | 1.93                     | 0.67              |
| 43:BU:8:VAL:CG1    | 43:BU:12:ARG:HE    | 2.07                     | 0.67              |
| 48:BZ:8:TYR:CE2    | 48:BZ:34:ARG:HD2   | 2.29                     | 0.67              |
| 1:CA:1410:G:H2'    | 1:CA:1411:C:C6     | 2.30                     | 0.67              |
| 1:CA:1511:G:H2'    | 1:CA:1512:U:O4'    | 1.95                     | 0.67              |
| 1:CA:397:A:H5'     | 1:CA:398:C:OP1     | 1.93                     | 0.67              |
| 1:CA:542:G:H2'     | 1:CA:543:C:H6      | 1.60                     | 0.67              |
| 1:CA:596:C:O2'     | 1:CA:597:G:H5'     | 1.95                     | 0.67              |
| 1:CA:60:A:H5''     | 1:CA:331:G:H22     | 1.60                     | 0.67              |
| 1:CA:674:G:H2'     | 1:CA:675:A:C8      | 2.28                     | 0.67              |
| 4:CD:13:ARG:O      | 4:CD:15:GLU:N      | 2.26                     | 0.67              |
| 4:CD:198:VAL:CG1   | 4:CD:199:ASN:N     | 2.57                     | 0.67              |
| 4:CD:31:CYS:C      | 4:CD:33:MET:H      | 1.95                     | 0.67              |
| 5:CE:10:MET:HB2    | 5:CE:32:VAL:HG22   | 1.76                     | 0.67              |
| 9:CI:89:ASN:HB3    | 9:CI:92:TYR:CD1    | 2.30                     | 0.67              |
| 11:CK:73:MET:HG2   | 11:CK:103:LEU:HD23 | 1.75                     | 0.67              |
| 15:CO:2:PRO:HG2    | 15:CO:3:ILE:H      | 1.59                     | 0.67              |
| 1:CA:1014:A:H4'    | 19:CS:14:HIS:CD2   | 2.29                     | 0.67              |
| 27:DA:1506:C:H2'   | 27:DA:1506:C:O2    | 1.93                     | 0.67              |
| 27:DA:415:A:H2'    | 27:DA:416:C:C6     | 2.29                     | 0.67              |
| 27:DA:71:A:OP2     | 27:DA:71:A:H3'     | 1.94                     | 0.67              |
| 27:DA:90:U:H1'     | 27:DA:92:A:H8      | 1.59                     | 0.67              |
| 29:DC:82:LYS:HG2   | 29:DC:151:GLU:O    | 1.94                     | 0.67              |
| 31:DE:4:ILE:HG23   | 31:DE:4:ILE:O      | 1.94                     | 0.67              |
| 33:DG:69:ALA:N     | 33:DG:91:ARG:O     | 2.25                     | 0.67              |
| 37:DO:5:GLN:OE1    | 37:DO:5:GLN:HA     | 1.93                     | 0.67              |
| 37:DO:66:LYS:HD3   | 37:DO:80:ASP:HA    | 1.75                     | 0.67              |
| 38:DP:146:VAL:HG13 | 38:DP:147:LEU:N    | 2.10                     | 0.67              |
| 40:DR:51:LEU:HA    | 40:DR:54:LEU:HB2   | 1.75                     | 0.67              |
| 42:DT:80:SER:HB3   | 42:DT:81:PRO:HD2   | 1.76                     | 0.67              |
| 1:AA:1517:G:H2'    | 1:AA:1518:A:C8     | 2.30                     | 0.67              |
| 1:AA:425:G:O2'     | 1:AA:426:G:H5'     | 1.95                     | 0.67              |
| 2:AB:110:GLN:O     | 2:AB:110:GLN:NE2   | 2.27                     | 0.67              |
| 2:AB:24:TRP:CZ3    | 2:AB:26:PRO:HA     | 2.28                     | 0.67              |
| 2:AB:69:LEU:HD12   | 2:AB:70:PHE:N      | 2.10                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:182:ILE:HD11  | 3:AC:203:PHE:CD1   | 2.29                     | 0.67              |
| 4:AD:108:LEU:HD11  | 4:AD:174:LEU:HB3   | 1.76                     | 0.67              |
| 8:AH:10:LEU:HD22   | 8:AH:83:ILE:HD11   | 1.76                     | 0.67              |
| 18:AR:74:ARG:HD3   | 18:AR:81:PHE:CE1   | 2.30                     | 0.67              |
| 27:BA:2090:G:H21   | 50:B1:45:ASN:ND2   | 1.92                     | 0.67              |
| 27:BA:1210:A:C5'   | 27:BA:1212:G:H5'   | 2.24                     | 0.67              |
| 27:BA:1266:G:OP2   | 54:B5:19:ARG:NH1   | 2.28                     | 0.67              |
| 27:BA:1885:A:H8    | 27:BA:1885:A:H5'   | 1.59                     | 0.67              |
| 27:BA:244:A:O2'    | 38:BP:73:GLY:HA3   | 1.95                     | 0.67              |
| 27:BA:2637:U:C2'   | 27:BA:2638:G:H5'   | 2.25                     | 0.67              |
| 30:BD:166:GLN:HB3  | 30:BD:174:ILE:HG22 | 1.76                     | 0.67              |
| 31:BE:2:LYS:HA     | 31:BE:84:PHE:CE2   | 2.30                     | 0.67              |
| 31:BE:74:PRO:O     | 31:BE:75:VAL:O     | 2.12                     | 0.67              |
| 34:BH:107:VAL:O    | 34:BH:109:PHE:N    | 2.28                     | 0.67              |
| 38:BP:146:VAL:HG13 | 38:BP:147:LEU:N    | 2.08                     | 0.67              |
| 39:BQ:51:ARG:O     | 39:BQ:51:ARG:HG2   | 1.94                     | 0.67              |
| 44:BV:18:LEU:HD22  | 44:BV:19:LYS:N     | 2.10                     | 0.67              |
| 47:BY:27:VAL:HG12  | 47:BY:29:GLU:H     | 1.59                     | 0.67              |
| 1:CA:967:C:H2'     | 1:CA:968:A:C8      | 2.30                     | 0.67              |
| 3:CC:73:PRO:C      | 3:CC:75:VAL:H      | 1.97                     | 0.67              |
| 3:CC:90:GLU:OE1    | 3:CC:93:LYS:HD3    | 1.95                     | 0.67              |
| 5:CE:12:LEU:HD22   | 5:CE:13:ILE:N      | 2.10                     | 0.67              |
| 10:CJ:94:VAL:HG12  | 10:CJ:95:GLU:H     | 1.60                     | 0.67              |
| 15:CO:54:ARG:O     | 15:CO:58:MET:HG3   | 1.94                     | 0.67              |
| 20:CT:72:LEU:O     | 20:CT:73:HIS:HB2   | 1.93                     | 0.67              |
| 49:D0:82:ARG:O     | 49:D0:82:ARG:HG3   | 1.93                     | 0.67              |
| 27:DA:15:G:H2'     | 27:DA:16:G:H8      | 1.58                     | 0.67              |
| 27:DA:1922:G:H2'   | 27:DA:1923:U:H6    | 1.60                     | 0.67              |
| 27:DA:2109:U:H2'   | 27:DA:2110:G:C8    | 2.29                     | 0.67              |
| 29:DC:58:VAL:CG2   | 29:DC:166:ASP:H    | 2.08                     | 0.67              |
| 30:DD:35:LYS:HZ1   | 30:DD:104:TYR:HB2  | 1.59                     | 0.67              |
| 30:DD:35:LYS:HB2   | 30:DD:36:PRO:HD3   | 1.76                     | 0.67              |
| 31:DE:39:PRO:HG3   | 31:DE:45:THR:OG1   | 1.95                     | 0.67              |
| 33:DG:15:VAL:HG22  | 33:DG:175:LEU:HB3  | 1.77                     | 0.67              |
| 34:DH:93:GLY:O     | 34:DH:94:TYR:HD1   | 1.78                     | 0.67              |
| 37:DO:16:ALA:HA    | 37:DO:46:ALA:HB1   | 1.77                     | 0.67              |
| 32:DF:187:VAL:HG12 | 38:DP:7:ARG:HH21   | 1.60                     | 0.67              |
| 8:AH:20:TYR:HA     | 8:AH:65:TYR:CE2    | 2.27                     | 0.67              |
| 8:AH:32:LYS:HA     | 8:AH:35:ILE:HD12   | 1.75                     | 0.67              |
| 16:AP:82:GLN:O     | 16:AP:83:GLU:HB2   | 1.95                     | 0.67              |
| 23:AW:36:A:H2'     | 23:AW:37:U:O4'     | 1.95                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AX:40:C:H2'     | 24:AX:41:C:C6      | 2.30                     | 0.67              |
| 27:BA:1021:A:H2'   | 27:BA:1023:U:H5'   | 1.77                     | 0.67              |
| 27:BA:1274:A:N3    | 27:BA:1297:C:H1'   | 2.10                     | 0.67              |
| 27:BA:1673:U:H2'   | 27:BA:1674:G:H5''  | 1.75                     | 0.67              |
| 29:BC:68:LEU:HB3   | 29:BC:70:LYS:HE2   | 1.74                     | 0.67              |
| 32:BF:25:PRO:HG3   | 32:BF:119:ARG:CB   | 2.25                     | 0.67              |
| 35:BI:114:LEU:HD23 | 35:BI:130:TYR:CE1  | 2.29                     | 0.67              |
| 35:BI:90:GLY:N     | 35:BI:121:LYS:HZ2  | 1.93                     | 0.67              |
| 35:BI:131:LYS:HG3  | 35:BI:132:PRO:CD   | 2.24                     | 0.67              |
| 37:BO:119:PRO:HB2  | 42:BT:68:TYR:HE1   | 1.60                     | 0.67              |
| 42:BT:30:VAL:HG11  | 42:BT:84:GLN:NE2   | 2.09                     | 0.67              |
| 47:BY:7:VAL:CG2    | 47:BY:8:LYS:HZ3    | 2.07                     | 0.67              |
| 2:CB:35:GLU:O      | 2:CB:35:GLU:HG2    | 1.94                     | 0.67              |
| 13:CM:72:ALA:O     | 13:CM:75:ALA:HB3   | 1.94                     | 0.67              |
| 27:DA:1374:G:H2'   | 27:DA:1375:C:C6    | 2.29                     | 0.67              |
| 27:DA:1897:G:O2'   | 27:DA:1898:U:H5'   | 1.93                     | 0.67              |
| 27:DA:2453:A:H2'   | 27:DA:2454:G:C8    | 2.30                     | 0.67              |
| 27:DA:753:C:O2     | 27:DA:753:C:H2'    | 1.95                     | 0.67              |
| 39:DQ:112:GLU:HA   | 39:DQ:115:MET:HG3  | 1.76                     | 0.67              |
| 42:DT:98:LYS:HB3   | 42:DT:100:TYR:CE1  | 2.30                     | 0.67              |
| 42:DT:109:GLU:HA   | 42:DT:112:ARG:HH11 | 1.59                     | 0.67              |
| 44:DV:19:LYS:NZ    | 44:DV:20:LEU:H     | 1.92                     | 0.67              |
| 44:DV:38:LEU:C     | 44:DV:39:LEU:HD13  | 2.15                     | 0.67              |
| 27:DA:565:C:H5     | 44:DV:78:LYS:HZ1   | 1.43                     | 0.67              |
| 45:DW:68:ARG:HA    | 45:DW:110:LYS:HD3  | 1.75                     | 0.67              |
| 1:AA:503:C:H2'     | 1:AA:504:C:H6      | 1.59                     | 0.67              |
| 1:AA:737:A:H2'     | 1:AA:738:C:C6      | 2.29                     | 0.67              |
| 5:AE:76:ILE:CG1    | 5:AE:77:PRO:HD2    | 2.24                     | 0.67              |
| 9:AI:102:LEU:O     | 9:AI:103:THR:OG1   | 2.11                     | 0.67              |
| 12:AL:116:LYS:O    | 12:AL:117:TYR:HB2  | 1.95                     | 0.67              |
| 12:AL:3:THR:O      | 12:AL:6:GLN:HB2    | 1.95                     | 0.67              |
| 15:AO:24:SER:O     | 15:AO:28:GLN:HG3   | 1.94                     | 0.67              |
| 27:BA:1605:C:H2'   | 27:BA:1606:G:O4'   | 1.95                     | 0.67              |
| 27:BA:1798:U:H5'   | 30:BD:259:THR:CG2  | 2.24                     | 0.67              |
| 27:BA:2147:G:H2'   | 27:BA:2148:G:O4'   | 1.95                     | 0.67              |
| 27:BA:327:G:H2'    | 27:BA:328:U:H6     | 1.58                     | 0.67              |
| 27:BA:814:C:H41    | 38:BP:27:HIS:CD2   | 2.12                     | 0.67              |
| 27:BA:2302:G:H21   | 33:BG:128:ARG:HG3  | 1.59                     | 0.67              |
| 34:BH:101:ARG:HB3  | 34:BH:117:PRO:HG3  | 1.77                     | 0.67              |
| 42:BT:89:VAL:HG21  | 42:BT:91:ARG:NH2   | 2.08                     | 0.67              |
| 43:BU:104:GLN:O    | 43:BU:107:ALA:HB3  | 1.94                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BU:75:ASN:O     | 43:BU:77:SER:N     | 2.28                     | 0.67              |
| 1:CA:1014:A:H2'    | 1:CA:1015:A:C8     | 2.30                     | 0.67              |
| 2:CB:23:ARG:HG2    | 2:CB:23:ARG:O      | 1.95                     | 0.67              |
| 7:CG:84:ASN:H      | 7:CG:84:ASN:ND2    | 1.93                     | 0.67              |
| 13:CM:76:ALA:HA    | 13:CM:79:LYS:CG    | 2.24                     | 0.67              |
| 15:CO:45:VAL:O     | 15:CO:47:LYS:HG2   | 1.95                     | 0.67              |
| 16:CP:18:ARG:HD3   | 16:CP:35:LYS:HD2   | 1.75                     | 0.67              |
| 20:CT:75:ASN:O     | 20:CT:78:ALA:N     | 2.28                     | 0.67              |
| 27:DA:2199:A:C2    | 27:DA:2200:C:H1'   | 2.30                     | 0.67              |
| 27:DA:552:G:H1'    | 27:DA:1220:A:C2    | 2.30                     | 0.67              |
| 30:DD:44:ASN:HB3   | 30:DD:49:ILE:HA    | 1.77                     | 0.67              |
| 36:DN:34:LEU:CD1   | 36:DN:120:LEU:HD23 | 2.20                     | 0.67              |
| 37:DO:14:THR:O     | 37:DO:52:VAL:HG12  | 1.94                     | 0.67              |
| 43:DU:72:HIS:ND1   | 43:DU:110:VAL:HG21 | 2.10                     | 0.67              |
| 1:AA:1327:C:O2'    | 1:AA:1328:C:H5'    | 1.94                     | 0.67              |
| 1:AA:1412:C:H2'    | 1:AA:1413:A:C8     | 2.30                     | 0.67              |
| 1:AA:609:A:C2'     | 1:AA:610:G:H5'     | 2.24                     | 0.67              |
| 4:AD:178:VAL:C     | 4:AD:180:GLY:H     | 1.99                     | 0.67              |
| 7:AG:154:TYR:O     | 7:AG:156:TRP:N     | 2.27                     | 0.67              |
| 7:AG:41:ARG:HH11   | 7:AG:41:ARG:HG2    | 1.60                     | 0.67              |
| 8:AH:64:LYS:C      | 8:AH:65:TYR:HD1    | 1.98                     | 0.67              |
| 13:AM:110:ARG:HH11 | 13:AM:110:ARG:HG2  | 1.60                     | 0.67              |
| 17:AQ:9:VAL:HG11   | 17:AQ:84:LEU:HD12  | 1.77                     | 0.67              |
| 27:BA:1665:A:O2'   | 27:BA:1666:G:H5'   | 1.95                     | 0.67              |
| 27:BA:2790:A:N3    | 27:BA:2791:C:H5''  | 2.10                     | 0.67              |
| 27:BA:539:G:H2'    | 27:BA:540:C:C6     | 2.30                     | 0.67              |
| 32:BF:2:LYS:O      | 32:BF:24:LEU:HB3   | 1.95                     | 0.67              |
| 40:BR:20:LEU:HD12  | 40:BR:24:GLN:HG3   | 1.75                     | 0.67              |
| 42:BT:31:SER:HB2   | 42:BT:32:TYR:CE2   | 2.30                     | 0.67              |
| 1:CA:560:U:H5'     | 1:CA:566:G:N2      | 2.10                     | 0.67              |
| 2:CB:36:ARG:H      | 2:CB:41:ILE:HD13   | 1.58                     | 0.67              |
| 4:CD:200:GLU:O     | 4:CD:203:VAL:HB    | 1.94                     | 0.67              |
| 13:CM:89:GLY:O     | 13:CM:93:ARG:HD2   | 1.95                     | 0.67              |
| 21:CU:6:ARG:HD3    | 21:CU:15:ARG:HH12  | 1.59                     | 0.67              |
| 55:D6:51:GLU:O     | 55:D6:52:VAL:HB    | 1.95                     | 0.67              |
| 27:DA:1164:G:H1    | 27:DA:1185:C:H42   | 1.41                     | 0.67              |
| 27:DA:173:G:H2'    | 27:DA:174:C:H6     | 1.60                     | 0.67              |
| 27:DA:1754:C:OP1   | 42:DT:96:ARG:NH1   | 2.27                     | 0.67              |
| 27:DA:2136:C:H2'   | 27:DA:2137:C:H6    | 1.60                     | 0.67              |
| 27:DA:2580:U:H4'   | 31:DE:130:GLY:HA3  | 1.76                     | 0.67              |
| 27:DA:398:G:H2'    | 27:DA:399:G:C8     | 2.29                     | 0.67              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:864:G:C5     | 27:DA:865:C:H5    | 2.13                     | 0.67              |
| 27:DA:97:C:H2'     | 27:DA:98:G:H8     | 1.58                     | 0.67              |
| 32:DF:24:LEU:HB3   | 32:DF:25:PRO:HD2  | 1.76                     | 0.67              |
| 34:DH:158:HIS:O    | 34:DH:159:GLU:HB2 | 1.95                     | 0.67              |
| 37:DO:71:ARG:HB3   | 37:DO:72:PRO:CD   | 2.25                     | 0.67              |
| 38:DP:99:LEU:HA    | 38:DP:102:ARG:NH1 | 2.10                     | 0.67              |
| 45:DW:27:LYS:O     | 45:DW:71:VAL:HG23 | 1.95                     | 0.67              |
| 46:DX:12:VAL:HG12  | 46:DX:27:THR:HG23 | 1.77                     | 0.67              |
| 47:DY:61:ILE:O     | 47:DY:62:GLU:HB2  | 1.94                     | 0.67              |
| 4:AD:146:ILE:H     | 4:AD:146:ILE:CD1  | 2.07                     | 0.66              |
| 10:AJ:48:THR:HA    | 10:AJ:62:HIS:CB   | 2.26                     | 0.66              |
| 13:AM:86:CYS:HA    | 19:AS:73:GLU:O    | 1.94                     | 0.66              |
| 23:AW:4:G:H2'      | 23:AW:5:G:O4'     | 1.95                     | 0.66              |
| 27:BA:1192:G:H2'   | 27:BA:1193:G:C5'  | 2.24                     | 0.66              |
| 27:BA:1916:A:H3'   | 27:BA:1917:U:H6   | 1.60                     | 0.66              |
| 27:BA:2386:C:H2'   | 27:BA:2387:U:C6   | 2.30                     | 0.66              |
| 27:BA:2416:C:H6    | 27:BA:2416:C:O5'  | 1.78                     | 0.66              |
| 27:BA:2542:A:H5'   | 27:BA:2543:G:OP1  | 1.94                     | 0.66              |
| 27:BA:2587:A:H2'   | 27:BA:2588:G:H5'  | 1.76                     | 0.66              |
| 27:BA:718:A:H3'    | 27:BA:719:C:C6    | 2.29                     | 0.66              |
| 33:BG:102:PHE:HA   | 33:BG:105:LYS:HZ2 | 1.59                     | 0.66              |
| 35:BI:120:ILE:HG22 | 35:BI:121:LYS:N   | 2.09                     | 0.66              |
| 44:BV:22:VAL:O     | 44:BV:23:GLU:HB2  | 1.95                     | 0.66              |
| 44:BV:40:LEU:H     | 44:BV:47:VAL:HG13 | 1.58                     | 0.66              |
| 44:BV:35:LEU:HB2   | 44:BV:57:VAL:CG1  | 2.25                     | 0.66              |
| 45:BW:62:HIS:O     | 45:BW:64:MET:HG3  | 1.95                     | 0.66              |
| 48:BZ:27:MET:HA    | 48:BZ:87:PHE:O    | 1.95                     | 0.66              |
| 1:CA:1266:G:H2'    | 1:CA:1268:A:OP2   | 1.95                     | 0.66              |
| 1:CA:321:A:H4'     | 1:CA:1436:U:H4'   | 1.77                     | 0.66              |
| 3:CC:71:ALA:HA     | 3:CC:105:GLU:HG3  | 1.77                     | 0.66              |
| 13:CM:76:ALA:HA    | 13:CM:79:LYS:HB2  | 1.76                     | 0.66              |
| 15:CO:74:ASP:OD2   | 15:CO:76:GLU:HB3  | 1.95                     | 0.66              |
| 19:CS:16:LEU:O     | 19:CS:20:LEU:HG   | 1.96                     | 0.66              |
| 56:D7:25:PRO:HG3   | 56:D7:28:ARG:HH22 | 1.60                     | 0.66              |
| 27:DA:987:G:O2'    | 27:DA:1000:A:N3   | 2.20                     | 0.66              |
| 27:DA:1339:G:H21   | 27:DA:1603:A:H1'  | 1.59                     | 0.66              |
| 27:DA:2704:C:H2'   | 27:DA:2705:A:C8   | 2.30                     | 0.66              |
| 32:DF:102:PRO:HB2  | 32:DF:105:VAL:CG2 | 2.26                     | 0.66              |
| 35:DI:129:THR:O    | 35:DI:130:TYR:HB2 | 1.95                     | 0.66              |
| 40:DR:117:VAL:O    | 40:DR:118:GLU:HB2 | 1.93                     | 0.66              |
| 41:DS:90:GLY:O     | 41:DS:92:TYR:N    | 2.28                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:DU:47:TYR:HD1  | 43:DU:50:ARG:HH22 | 1.44                     | 0.66              |
| 44:DV:5:VAL:HG23  | 44:DV:37:VAL:CG2  | 2.26                     | 0.66              |
| 1:AA:1113:C:H2'   | 1:AA:1114:C:H6    | 1.60                     | 0.66              |
| 1:AA:1146:A:C2'   | 1:AA:1147:C:H5''  | 2.25                     | 0.66              |
| 2:AB:56:ARG:O     | 2:AB:60:ASP:HB2   | 1.95                     | 0.66              |
| 8:AH:25:ASP:OD1   | 8:AH:25:ASP:N     | 2.28                     | 0.66              |
| 9:AI:96:LEU:HD11  | 9:AI:102:LEU:HD23 | 1.75                     | 0.66              |
| 16:AP:15:PRO:O    | 16:AP:16:HIS:ND1  | 2.28                     | 0.66              |
| 55:B6:32:ASN:CG   | 55:B6:33:LYS:H    | 1.98                     | 0.66              |
| 27:BA:2183:C:H2'  | 27:BA:2184:G:H8   | 1.59                     | 0.66              |
| 30:BD:72:LYS:CD   | 30:BD:75:ILE:HD12 | 2.24                     | 0.66              |
| 27:BA:2052:G:N3   | 31:BE:149:ARG:HA  | 2.10                     | 0.66              |
| 37:BO:108:GLU:C   | 37:BO:110:GLY:H   | 1.99                     | 0.66              |
| 37:BO:12:ASP:OD2  | 37:BO:14:THR:HB   | 1.95                     | 0.66              |
| 40:BR:53:HIS:HD2  | 40:BR:94:TYR:OH   | 1.78                     | 0.66              |
| 42:BT:27:THR:O    | 42:BT:28:VAL:CG2  | 2.35                     | 0.66              |
| 47:BY:97:ARG:C    | 47:BY:98:VAL:HG23 | 2.14                     | 0.66              |
| 2:CB:178:ARG:HH22 | 8:CH:68:ARG:NH2   | 1.93                     | 0.66              |
| 3:CC:73:PRO:HA    | 3:CC:76:VAL:HG22  | 1.76                     | 0.66              |
| 11:CK:21:ILE:HD12 | 11:CK:21:ILE:N    | 2.09                     | 0.66              |
| 49:D0:48:GLY:HA3  | 49:D0:80:HIS:ND1  | 2.10                     | 0.66              |
| 27:DA:2755:C:H3'  | 58:D9:19:ARG:HH21 | 1.60                     | 0.66              |
| 27:DA:2862:G:O2'  | 27:DA:2863:C:H5'  | 1.95                     | 0.66              |
| 27:DA:412:A:C8    | 27:DA:412:A:H5'   | 2.29                     | 0.66              |
| 27:DA:529:A:H5''  | 27:DA:530:G:OP1   | 1.96                     | 0.66              |
| 27:DA:714:U:H2'   | 27:DA:715:G:H5''  | 1.76                     | 0.66              |
| 27:DA:867:C:H2'   | 27:DA:868:U:C6    | 2.30                     | 0.66              |
| 36:DN:25:ARG:CG   | 36:DN:25:ARG:HH11 | 2.08                     | 0.66              |
| 27:DA:1275:A:C8   | 40:DR:16:HIS:HD2  | 2.13                     | 0.66              |
| 40:DR:8:ARG:HE    | 40:DR:8:ARG:HA    | 1.60                     | 0.66              |
| 45:DW:24:ILE:O    | 45:DW:71:VAL:HG21 | 1.95                     | 0.66              |
| 48:DZ:60:LEU:CB   | 48:DZ:64:GLN:HB2  | 2.25                     | 0.66              |
| 1:AA:619:U:H6     | 1:AA:619:U:O5'    | 1.78                     | 0.66              |
| 1:AA:737:A:H2'    | 1:AA:738:C:H6     | 1.58                     | 0.66              |
| 2:AB:141:GLU:O    | 2:AB:145:LEU:HD23 | 1.95                     | 0.66              |
| 4:AD:8:VAL:HB     | 4:AD:22:LYS:HZ1   | 1.60                     | 0.66              |
| 11:AK:48:ILE:CD1  | 11:AK:64:ALA:HA   | 2.25                     | 0.66              |
| 23:AW:30:A:C3'    | 23:AW:31:U:H5''   | 2.24                     | 0.66              |
| 27:BA:1171:G:H3'  | 27:BA:1173:G:H4'  | 1.76                     | 0.66              |
| 27:BA:2037:G:H2'  | 27:BA:2038:G:H8   | 1.58                     | 0.66              |
| 27:BA:2057:A:H2'  | 27:BA:2058:A:O4'  | 1.96                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2340:G:O2'   | 27:BA:2341:G:H5'   | 1.94                     | 0.66              |
| 27:BA:626:U:C5'    | 27:BA:627:A:H5'    | 2.25                     | 0.66              |
| 30:BD:60:ARG:HE    | 30:BD:86:PRO:HB2   | 1.59                     | 0.66              |
| 32:BF:192:LEU:HD23 | 32:BF:193:VAL:N    | 2.11                     | 0.66              |
| 33:BG:35:GLU:HB2   | 33:BG:160:VAL:O    | 1.94                     | 0.66              |
| 48:BZ:149:LEU:O    | 48:BZ:170:ILE:HD11 | 1.96                     | 0.66              |
| 1:CA:997:U:H2'     | 1:CA:998:G:C8      | 2.30                     | 0.66              |
| 3:CC:113:ALA:HB2   | 3:CC:202:ILE:HG13  | 1.78                     | 0.66              |
| 11:CK:123:LYS:O    | 11:CK:126:ARG:HB2  | 1.95                     | 0.66              |
| 50:D1:3:LYS:HG3    | 50:D1:4:VAL:H      | 1.58                     | 0.66              |
| 53:D4:48:ILE:H     | 53:D4:48:ILE:HD12  | 1.59                     | 0.66              |
| 32:DF:108:LYS:O    | 32:DF:112:MET:N    | 2.25                     | 0.66              |
| 32:DF:157:VAL:HB   | 32:DF:194:MET:CB   | 2.24                     | 0.66              |
| 33:DG:15:VAL:HG13  | 33:DG:175:LEU:HD22 | 1.76                     | 0.66              |
| 38:DP:71:VAL:CG1   | 38:DP:72:PRO:HD3   | 2.09                     | 0.66              |
| 45:DW:29:LEU:HD12  | 45:DW:29:LEU:O     | 1.95                     | 0.66              |
| 10:AJ:5:ARG:HA     | 10:AJ:73:ASP:OD1   | 1.95                     | 0.66              |
| 27:BA:1936:A:H3'   | 27:BA:1937:A:H5''  | 1.78                     | 0.66              |
| 31:BE:75:VAL:HG12  | 31:BE:76:ARG:H     | 1.60                     | 0.66              |
| 33:BG:109:VAL:C    | 33:BG:112:PRO:HD2  | 2.16                     | 0.66              |
| 34:BH:32:GLU:O     | 34:BH:33:LEU:HD23  | 1.96                     | 0.66              |
| 39:BQ:26:TYR:HD1   | 39:BQ:28:ALA:HB2   | 1.58                     | 0.66              |
| 46:BX:31:HIS:CD2   | 46:BX:33:LYS:H     | 2.14                     | 0.66              |
| 1:CA:193:C:C2'     | 1:CA:194:C:H5'     | 2.25                     | 0.66              |
| 1:CA:227:G:H2'     | 1:CA:228:A:H8      | 1.60                     | 0.66              |
| 5:CE:12:LEU:HD13   | 5:CE:12:LEU:C      | 2.16                     | 0.66              |
| 8:CH:109:ILE:HD11  | 8:CH:120:THR:HG21  | 1.77                     | 0.66              |
| 23:CW:42:G:H3'     | 23:CW:43:C:C5'     | 2.24                     | 0.66              |
| 56:D7:29:LYS:HG2   | 56:D7:33:ARG:HH21  | 1.60                     | 0.66              |
| 58:D9:15:LYS:HE2   | 58:D9:17:ILE:CD1   | 2.21                     | 0.66              |
| 30:DD:111:LEU:HD13 | 30:DD:112:GLN:N    | 2.09                     | 0.66              |
| 27:DA:1658:C:OP1   | 31:DE:132:HIS:O    | 2.13                     | 0.66              |
| 31:DE:32:PRO:HA    | 31:DE:90:THR:HA    | 1.76                     | 0.66              |
| 38:DP:144:GLU:H    | 38:DP:145:PRO:CD   | 2.07                     | 0.66              |
| 38:DP:38:GLN:HG3   | 38:DP:39:LYS:N     | 2.10                     | 0.66              |
| 39:DQ:98:LYS:HB3   | 39:DQ:99:PRO:CD    | 2.25                     | 0.66              |
| 1:AA:174:C:H2'     | 1:AA:175:C:C6      | 2.30                     | 0.66              |
| 1:AA:967:C:OP2     | 1:AA:969:A:H5'     | 1.95                     | 0.66              |
| 11:AK:126:ARG:NH1  | 11:AK:126:ARG:HB3  | 2.09                     | 0.66              |
| 6:AF:49:ALA:HB1    | 18:AR:80:PRO:HB3   | 1.76                     | 0.66              |
| 27:BA:1195:G:O2'   | 27:BA:1196:C:H5'   | 1.95                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:271(P):C:H5' | 27:BA:271(P):C:H6  | 1.61                     | 0.66              |
| 27:BA:922:U:H2'    | 27:BA:923:C:H6     | 1.58                     | 0.66              |
| 28:BB:105:A:H2'    | 28:BB:106:G:C5'    | 2.25                     | 0.66              |
| 34:BH:10:PRO:HG2   | 34:BH:50:VAL:H     | 1.58                     | 0.66              |
| 35:BI:84:GLY:O     | 35:BI:85:GLU:HB2   | 1.96                     | 0.66              |
| 36:BN:85:ILE:HG21  | 36:BN:90:MET:CE    | 2.25                     | 0.66              |
| 38:BP:17:LYS:CG    | 38:BP:19:VAL:HG23  | 2.25                     | 0.66              |
| 39:BQ:65:PHE:HB2   | 39:BQ:105:GLU:HG2  | 1.77                     | 0.66              |
| 46:BX:92:LEU:O     | 46:BX:94:GLY:N     | 2.25                     | 0.66              |
| 1:CA:221:C:O2'     | 1:CA:222:U:H5'     | 1.96                     | 0.66              |
| 9:CI:77:ILE:O      | 9:CI:81:ILE:HG12   | 1.95                     | 0.66              |
| 24:CX:23:C:H2'     | 24:CX:24:U:H6      | 1.60                     | 0.66              |
| 25:CY:2:G:H1       | 25:CY:70:C:N4      | 1.92                     | 0.66              |
| 27:DA:2392:A:OP2   | 57:D8:31:HIS:HE1   | 1.78                     | 0.66              |
| 27:DA:1221(A):C:N4 | 27:DA:1228:G:H1    | 1.92                     | 0.66              |
| 27:DA:2575:C:H2'   | 27:DA:2578:G:O6    | 1.95                     | 0.66              |
| 27:DA:271(U):G:O2' | 27:DA:271(V):G:H5' | 1.96                     | 0.66              |
| 30:DD:58:HIS:CD2   | 30:DD:59:LYS:O     | 2.47                     | 0.66              |
| 27:DA:2511:U:O3'   | 31:DE:123:ALA:HB3  | 1.96                     | 0.66              |
| 32:DF:187:VAL:C    | 38:DP:7:ARG:HH22   | 1.98                     | 0.66              |
| 39:DQ:10:ARG:HG3   | 39:DQ:10:ARG:NH1   | 2.10                     | 0.66              |
| 27:DA:908:C:OP2    | 39:DQ:22:LYS:HD2   | 1.95                     | 0.66              |
| 42:DT:118:ARG:HB3  | 42:DT:122:ASP:OD1  | 1.95                     | 0.66              |
| 47:DY:88:LYS:CE    | 47:DY:93:GLY:HA3   | 2.25                     | 0.66              |
| 1:AA:565:U:H3'     | 1:AA:566:G:H2'     | 1.78                     | 0.66              |
| 2:AB:42:ILE:CD1    | 2:AB:202:PRO:HB2   | 2.24                     | 0.66              |
| 9:AI:70:LYS:O      | 9:AI:74:ILE:HG13   | 1.95                     | 0.66              |
| 15:AO:81:LEU:HG    | 15:AO:82:ILE:N     | 2.10                     | 0.66              |
| 27:BA:54:G:O2'     | 56:B7:35:ARG:HD3   | 1.95                     | 0.66              |
| 27:BA:1346:G:H2'   | 27:BA:1347:G:H8    | 1.60                     | 0.66              |
| 27:BA:2419:U:H5'   | 55:B6:23:THR:HG21  | 1.77                     | 0.66              |
| 30:BD:158:ALA:HB3  | 30:BD:161:THR:HG21 | 1.76                     | 0.66              |
| 31:BE:21:VAL:O     | 31:BE:23:VAL:HG13  | 1.95                     | 0.66              |
| 32:BF:181:LEU:HB3  | 32:BF:205:ARG:HH12 | 1.58                     | 0.66              |
| 34:BH:19:VAL:HG21  | 34:BH:44:VAL:HA    | 1.76                     | 0.66              |
| 38:BP:89:ALA:HA    | 38:BP:121:LYS:CD   | 2.25                     | 0.66              |
| 47:BY:11:ASP:N     | 47:BY:27:VAL:HG22  | 2.11                     | 0.66              |
| 1:CA:1065:U:H5''   | 1:CA:1190:G:N2     | 2.10                     | 0.66              |
| 1:CA:762:C:O2'     | 1:CA:763:G:H5'     | 1.96                     | 0.66              |
| 1:CA:853:G:O2'     | 1:CA:854:G:H5'     | 1.95                     | 0.66              |
| 3:CC:64:VAL:HG22   | 3:CC:99:VAL:HA     | 1.77                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CK:78:GLN:O     | 11:CK:103:LEU:HD13 | 1.95                     | 0.66              |
| 12:CL:22:PRO:C     | 12:CL:24:LEU:H     | 1.96                     | 0.66              |
| 10:CJ:53:PRO:HA    | 14:CN:42:ILE:HD13  | 1.77                     | 0.66              |
| 27:DA:931:G:O2'    | 52:D3:24:LYS:HD2   | 1.95                     | 0.66              |
| 55:D6:10:LEU:H     | 55:D6:10:LEU:HD23  | 1.59                     | 0.66              |
| 27:DA:1264:G:H5'   | 54:D5:11:THR:OG1   | 1.95                     | 0.66              |
| 27:DA:1895:C:O2'   | 27:DA:1896:G:H5'   | 1.96                     | 0.66              |
| 31:DE:51:PHE:CD1   | 31:DE:52:LEU:N     | 2.64                     | 0.66              |
| 27:DA:2787:C:C1'   | 31:DE:61:ARG:HG3   | 2.21                     | 0.66              |
| 32:DF:109:GLY:O    | 32:DF:113:ALA:N    | 2.22                     | 0.66              |
| 34:DH:58:GLU:O     | 34:DH:62:LYS:HG3   | 1.94                     | 0.66              |
| 37:DO:16:ALA:HB2   | 37:DO:52:VAL:HG11  | 1.78                     | 0.66              |
| 1:AA:1022:G:H2'    | 1:AA:1023:G:H8     | 1.60                     | 0.66              |
| 1:AA:1108:G:OP2    | 3:AC:174:PRO:HA    | 1.96                     | 0.66              |
| 1:AA:1116:C:C2'    | 1:AA:1117:G:H5'    | 2.24                     | 0.66              |
| 1:AA:559:A:H4'     | 1:AA:560:U:O5'     | 1.96                     | 0.66              |
| 4:AD:146:ILE:HD12  | 4:AD:146:ILE:N     | 2.11                     | 0.66              |
| 15:AO:18:PHE:CD1   | 15:AO:18:PHE:O     | 2.48                     | 0.66              |
| 50:B1:93:GLU:C     | 50:B1:95:LEU:H     | 1.99                     | 0.66              |
| 27:BA:1316:U:H2'   | 27:BA:1317:A:H8    | 1.59                     | 0.66              |
| 27:BA:194:G:H2'    | 27:BA:195:A:O4'    | 1.95                     | 0.66              |
| 27:BA:1991:U:H5''  | 27:BA:1991:U:H6    | 1.60                     | 0.66              |
| 27:BA:2117:A:O2'   | 27:BA:2118:U:H3'   | 1.95                     | 0.66              |
| 27:BA:2787:C:O2    | 27:BA:2787:C:H2'   | 1.95                     | 0.66              |
| 30:BD:76:PRO:HG2   | 30:BD:98:VAL:HG21  | 1.76                     | 0.66              |
| 39:BQ:57:HIS:CE1   | 39:BQ:116:GLU:HG2  | 2.31                     | 0.66              |
| 45:BW:28:SER:OG    | 45:BW:31:GLU:HB2   | 1.96                     | 0.66              |
| 47:BY:85:VAL:HG13  | 47:BY:92:ASN:OD1   | 1.95                     | 0.66              |
| 48:BZ:149:LEU:HD23 | 48:BZ:170:ILE:CG1  | 2.22                     | 0.66              |
| 1:CA:187:C:H5'     | 20:CT:82:SER:HA    | 1.78                     | 0.66              |
| 1:CA:831:U:C2'     | 1:CA:832:C:H5'     | 2.25                     | 0.66              |
| 5:CE:13:ILE:HA     | 5:CE:29:GLY:O      | 1.95                     | 0.66              |
| 19:CS:61:TYR:O     | 19:CS:62:ILE:HB    | 1.95                     | 0.66              |
| 27:DA:227:A:H61    | 27:DA:410:G:N2     | 1.92                     | 0.66              |
| 27:DA:993:G:H1'    | 44:DV:89:GLN:HG3   | 1.78                     | 0.66              |
| 32:DF:24:LEU:O     | 32:DF:26:ALA:N     | 2.28                     | 0.66              |
| 33:DG:107:LEU:HD11 | 33:DG:178:PHE:CE1  | 2.30                     | 0.66              |
| 40:DR:14:SER:O     | 40:DR:16:HIS:N     | 2.28                     | 0.66              |
| 43:DU:65:ILE:HD11  | 43:DU:96:ALA:HB3   | 1.77                     | 0.66              |
| 44:DV:2:PHE:O      | 44:DV:14:VAL:O     | 2.13                     | 0.66              |
| 27:DA:896:A:H2     | 48:DZ:113:GLY:HA3  | 1.61                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1100:C:O2    | 1:AA:1102:A:H5'    | 1.96                     | 0.66              |
| 1:AA:189(E):U:O2' | 1:AA:189(F):U:H5'' | 1.96                     | 0.66              |
| 1:AA:109:A:H2'    | 1:AA:326:G:H21     | 1.59                     | 0.66              |
| 1:AA:332:G:O2'    | 1:AA:333:G:H5'     | 1.96                     | 0.66              |
| 1:AA:76:C:H42     | 1:AA:93:G:H1       | 1.41                     | 0.66              |
| 3:AC:114:PRO:HD3  | 3:AC:184:TYR:O     | 1.96                     | 0.66              |
| 3:AC:58:GLU:H     | 3:AC:65:ALA:HB3    | 1.61                     | 0.66              |
| 8:AH:6:ILE:HD13   | 8:AH:85:ARG:HH22   | 1.59                     | 0.66              |
| 9:AI:97:LYS:HB3   | 9:AI:98:PRO:HD3    | 1.77                     | 0.66              |
| 17:AQ:43:LEU:CD1  | 17:AQ:68:ARG:HG2   | 2.24                     | 0.66              |
| 23:AW:63:C:H2'    | 23:AW:64:G:H8      | 1.59                     | 0.66              |
| 27:BA:1588:C:O2   | 27:BA:1588:C:H2'   | 1.96                     | 0.66              |
| 27:BA:2682:U:H6   | 27:BA:2682:U:H5'   | 1.60                     | 0.66              |
| 27:BA:635:C:H2'   | 27:BA:636:G:C8     | 2.29                     | 0.66              |
| 27:BA:673:C:C2'   | 27:BA:674:G:H5'    | 2.25                     | 0.66              |
| 27:BA:718:A:H3'   | 27:BA:719:C:H6     | 1.60                     | 0.66              |
| 27:BA:762:U:H4'   | 27:BA:763:G:O5'    | 1.95                     | 0.66              |
| 28:BB:105:A:C2'   | 28:BB:106:G:H5'    | 2.26                     | 0.66              |
| 31:BE:46:ALA:CB   | 31:BE:82:ARG:HA    | 2.24                     | 0.66              |
| 32:BF:20:LEU:CD1  | 32:BF:203:GLN:HE22 | 2.08                     | 0.66              |
| 32:BF:3:GLU:CB    | 32:BF:24:LEU:HG    | 2.26                     | 0.66              |
| 33:BG:91:ARG:C    | 33:BG:91:ARG:HD2   | 2.16                     | 0.66              |
| 27:BA:2415:G:H4'  | 38:BP:67:MET:H     | 1.61                     | 0.66              |
| 39:BQ:57:HIS:HE1  | 39:BQ:116:GLU:HG2  | 1.61                     | 0.66              |
| 47:BY:87:LYS:HG3  | 47:BY:88:LYS:H     | 1.58                     | 0.66              |
| 1:CA:830:G:H1     | 1:CA:856:C:H42     | 1.44                     | 0.66              |
| 6:CF:78:GLU:O     | 6:CF:81:ILE:HG13   | 1.96                     | 0.66              |
| 10:CJ:8:LEU:CD2   | 10:CJ:96:ILE:HG22  | 2.25                     | 0.66              |
| 15:CO:87:ILE:HG22 | 15:CO:88:ARG:N     | 2.07                     | 0.66              |
| 19:CS:33:THR:OG1  | 19:CS:34:TRP:N     | 2.27                     | 0.66              |
| 56:D7:1:MET:N     | 56:D7:1:MET:SD     | 2.64                     | 0.66              |
| 58:D9:18:ARG:O    | 58:D9:18:ARG:HG3   | 1.94                     | 0.66              |
| 27:DA:1138:G:H2'  | 27:DA:1139:G:O4'   | 1.95                     | 0.66              |
| 27:DA:1314:C:N3   | 27:DA:1339:G:C2    | 2.64                     | 0.66              |
| 27:DA:1351:C:H2'  | 27:DA:1352:U:C6    | 2.31                     | 0.66              |
| 27:DA:1398:C:H5'  | 27:DA:1398:C:C6    | 2.30                     | 0.66              |
| 27:DA:1496:A:H2'  | 27:DA:1498:C:N4    | 2.11                     | 0.66              |
| 27:DA:2822:G:OP2  | 40:DR:2:ARG:NH1    | 2.29                     | 0.66              |
| 29:DC:36:LYS:HD3  | 29:DC:37:PHE:N     | 2.10                     | 0.66              |
| 31:DE:9:VAL:HG22  | 31:DE:10:GLY:N     | 2.10                     | 0.66              |
| 34:DH:68:THR:CG2  | 34:DH:72:ILE:HD11  | 2.26                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DP:123:LEU:CD1  | 38:DP:125:VAL:HG12 | 2.25                     | 0.66              |
| 38:DP:71:VAL:HG13  | 38:DP:72:PRO:CD    | 2.11                     | 0.66              |
| 46:DX:64:LYS:HZ2   | 46:DX:73:ARG:NH1   | 1.92                     | 0.66              |
| 48:DZ:156:LEU:HB3  | 48:DZ:160:VAL:HG12 | 1.78                     | 0.66              |
| 1:AA:578:C:O2'     | 1:AA:579:G:H8      | 1.79                     | 0.66              |
| 11:AK:13:GLN:OE1   | 11:AK:75:TYR:HA    | 1.95                     | 0.66              |
| 15:AO:7:GLU:O      | 15:AO:11:VAL:HG23  | 1.96                     | 0.66              |
| 57:B8:51:ALA:N     | 57:B8:53:PRO:HD2   | 2.09                     | 0.66              |
| 27:BA:1018:C:H2'   | 27:BA:1018:C:O2    | 1.96                     | 0.66              |
| 27:BA:1286:A:C2'   | 27:BA:1288:U:OP2   | 2.44                     | 0.66              |
| 27:BA:1476:C:H2'   | 27:BA:1477:A:H8    | 1.59                     | 0.66              |
| 29:BC:193:ILE:O    | 29:BC:195:ALA:N    | 2.28                     | 0.66              |
| 29:BC:19:VAL:HG12  | 29:BC:20:TYR:HD1   | 1.61                     | 0.66              |
| 30:BD:93:ALA:HB2   | 30:BD:107:ALA:HB2  | 1.77                     | 0.66              |
| 31:BE:184:VAL:CG1  | 31:BE:185:LYS:N    | 2.59                     | 0.66              |
| 32:BF:165:ARG:HA   | 32:BF:168:ARG:CD   | 2.24                     | 0.66              |
| 32:BF:20:LEU:HD22  | 32:BF:203:GLN:HE22 | 1.61                     | 0.66              |
| 37:BO:121:VAL:HG12 | 37:BO:121:VAL:O    | 1.96                     | 0.66              |
| 37:BO:13:ASN:N     | 37:BO:13:ASN:OD1   | 2.27                     | 0.66              |
| 38:BP:144:GLU:HG2  | 38:BP:144:GLU:O    | 1.96                     | 0.66              |
| 39:BQ:58:PHE:O     | 39:BQ:58:PHE:HD1   | 1.78                     | 0.66              |
| 43:BU:92:ARG:HG2   | 44:BV:11:GLN:NE2   | 2.10                     | 0.66              |
| 1:CA:1134:G:N2     | 1:CA:1141:C:C2     | 2.64                     | 0.66              |
| 1:CA:584:G:H2'     | 1:CA:585:G:C8      | 2.31                     | 0.66              |
| 1:CA:611:A:O2'     | 1:CA:612:C:H5'     | 1.96                     | 0.66              |
| 5:CE:94:ALA:HB3    | 5:CE:118:ILE:N     | 2.10                     | 0.66              |
| 14:CN:13:THR:N     | 14:CN:14:PRO:CD    | 2.59                     | 0.66              |
| 54:D5:41:PRO:HG2   | 54:D5:44:THR:OG1   | 1.95                     | 0.66              |
| 30:DD:25:THR:HG22  | 30:DD:26:LYS:H     | 1.61                     | 0.66              |
| 30:DD:62:TYR:HA    | 30:DD:87:ASN:HD21  | 1.60                     | 0.66              |
| 33:DG:142:PRO:HG2  | 33:DG:143:GLU:H    | 1.61                     | 0.66              |
| 33:DG:119:GLY:O    | 33:DG:181:ARG:NE   | 2.29                     | 0.66              |
| 35:DI:81:VAL:HG21  | 35:DI:142:VAL:CG1  | 2.26                     | 0.66              |
| 37:DO:101:PRO:HG2  | 42:DT:67:SER:HB3   | 1.77                     | 0.66              |
| 40:DR:13:HIS:ND1   | 40:DR:13:HIS:O     | 2.29                     | 0.66              |
| 48:DZ:124:LEU:HD12 | 48:DZ:125:VAL:H    | 1.61                     | 0.66              |
| 48:DZ:13:LYS:N     | 48:DZ:14:PRO:HD3   | 2.11                     | 0.66              |
| 1:AA:1067:A:H1'    | 1:AA:1068:G:O4'    | 1.95                     | 0.66              |
| 1:AA:1221:G:O2'    | 1:AA:1222:G:H5'    | 1.96                     | 0.66              |
| 1:AA:452:A:O2'     | 1:AA:453:A:H5''    | 1.95                     | 0.66              |
| 4:AD:156:GLU:O     | 4:AD:160:GLN:HG3   | 1.97                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:40:ARG:HB3    | 5:AE:66:MET:HE3    | 1.76                     | 0.66              |
| 12:AL:38:ARG:NH1   | 12:AL:54:LYS:NZ    | 2.44                     | 0.66              |
| 24:AX:29:G:O2'     | 24:AX:30:G:H5'     | 1.96                     | 0.66              |
| 54:B5:57:VAL:O     | 54:B5:58:LEU:HD23  | 1.96                     | 0.66              |
| 27:BA:1310:G:N2    | 27:BA:1313:U:C4    | 2.64                     | 0.66              |
| 27:BA:2200:C:H2'   | 27:BA:2201:C:C6    | 2.28                     | 0.66              |
| 27:BA:2267:A:N3    | 27:BA:2267:A:H2'   | 2.09                     | 0.66              |
| 27:BA:2732:G:C3'   | 27:BA:2733:A:H5'   | 2.25                     | 0.66              |
| 38:BP:48:PRO:CG    | 38:BP:49:ARG:H     | 2.09                     | 0.66              |
| 41:BS:48:LEU:N     | 41:BS:48:LEU:HD12  | 2.10                     | 0.66              |
| 41:BS:88:ASP:OD2   | 41:BS:89:ARG:N     | 2.29                     | 0.66              |
| 42:BT:13:ARG:C     | 42:BT:15:VAL:H     | 1.98                     | 0.66              |
| 36:BN:4:TYR:HB2    | 43:BU:64:ARG:HH12  | 1.60                     | 0.66              |
| 47:BY:99:CYS:SG    | 59:BY:201:MG:MG    | 1.79                     | 0.66              |
| 47:BY:31:LEU:HD23  | 47:BY:36:ALA:O     | 1.95                     | 0.66              |
| 48:BZ:150:HIS:CB   | 48:BZ:169:THR:HA   | 2.24                     | 0.66              |
| 1:CA:197:A:O2'     | 1:CA:198:G:C8      | 2.49                     | 0.66              |
| 1:CA:862:C:O4'     | 1:CA:874:G:H4'     | 1.96                     | 0.66              |
| 27:DA:1050:A:HO2'  | 27:DA:1051:G:H8    | 1.44                     | 0.66              |
| 27:DA:1174:A:H5''  | 27:DA:1175:U:H5'   | 1.77                     | 0.66              |
| 27:DA:1503:U:H2'   | 27:DA:1504:C:C6    | 2.28                     | 0.66              |
| 27:DA:1827:C:OP2   | 30:DD:222:ARG:NH1  | 2.28                     | 0.66              |
| 27:DA:2247:A:H2'   | 27:DA:2248:C:C6    | 2.30                     | 0.66              |
| 27:DA:251:A:H2'    | 27:DA:252:G:O4'    | 1.95                     | 0.66              |
| 27:DA:582:G:H2'    | 27:DA:583:G:C8     | 2.31                     | 0.66              |
| 27:DA:598:G:H5'    | 38:DP:15:ARG:HD2   | 1.76                     | 0.66              |
| 39:DQ:38:GLU:HG3   | 39:DQ:127:ILE:HB   | 1.78                     | 0.66              |
| 39:DQ:1:MET:HE1    | 39:DQ:44:ALA:HB1   | 1.77                     | 0.66              |
| 48:DZ:149:LEU:HD22 | 48:DZ:149:LEU:H    | 1.59                     | 0.66              |
| 1:AA:1030(B):C:H2' | 1:AA:1030(C):G:H5' | 1.78                     | 0.65              |
| 2:AB:172:ILE:H     | 2:AB:172:ILE:CD1   | 2.05                     | 0.65              |
| 3:AC:70:VAL:HG12   | 3:AC:72:LYS:H      | 1.61                     | 0.65              |
| 4:AD:189:PRO:HB2   | 4:AD:194:LEU:HD21  | 1.76                     | 0.65              |
| 6:AF:24:GLU:HG3    | 6:AF:25:ILE:N      | 2.11                     | 0.65              |
| 8:AH:107:LEU:H     | 8:AH:107:LEU:HD23  | 1.61                     | 0.65              |
| 11:AK:32:ILE:HG12  | 11:AK:41:THR:O     | 1.97                     | 0.65              |
| 13:AM:15:VAL:HG12  | 13:AM:45:VAL:CG2   | 2.26                     | 0.65              |
| 16:AP:6:LEU:HB3    | 16:AP:17:TYR:CB    | 2.26                     | 0.65              |
| 28:BB:91:C:H2'     | 28:BB:92:C:H6      | 1.61                     | 0.65              |
| 31:BE:50:GLY:HA2   | 31:BE:78:LEU:CB    | 2.26                     | 0.65              |
| 39:BQ:110:THR:HG23 | 39:BQ:113:GLN:CB   | 2.18                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BT:106:SER:HB3 | 42:BT:110:ILE:HD11 | 1.76                     | 0.65              |
| 47:BY:60:PHE:HA   | 47:BY:62:GLU:OE2   | 1.96                     | 0.65              |
| 47:BY:96:ILE:HD12 | 47:BY:99:CYS:CB    | 2.25                     | 0.65              |
| 1:CA:932:C:O2     | 1:CA:932:C:H2'     | 1.95                     | 0.65              |
| 8:CH:112:LEU:HA   | 8:CH:134:ILE:HG12  | 1.76                     | 0.65              |
| 10:CJ:48:THR:HA   | 10:CJ:62:HIS:HB2   | 1.78                     | 0.65              |
| 12:CL:5:ASN:HA    | 12:CL:8:VAL:CG2    | 2.26                     | 0.65              |
| 24:CX:73:A:H5'    | 24:CX:74:C:H5'     | 1.78                     | 0.65              |
| 27:DA:380:U:H2'   | 27:DA:381:G:C8     | 2.31                     | 0.65              |
| 27:DA:38:A:O2'    | 27:DA:39:C:H5'     | 1.96                     | 0.65              |
| 27:DA:763:G:N3    | 27:DA:765:G:H1'    | 2.10                     | 0.65              |
| 27:DA:783:A:H2'   | 27:DA:784:A:O5'    | 1.95                     | 0.65              |
| 31:DE:9:VAL:CG1   | 31:DE:25:VAL:HB    | 2.26                     | 0.65              |
| 34:DH:85:LYS:HD2  | 34:DH:141:VAL:HG13 | 1.77                     | 0.65              |
| 35:DI:77:LEU:HD23 | 35:DI:78:THR:N     | 2.11                     | 0.65              |
| 39:DQ:38:GLU:OE2  | 39:DQ:127:ILE:HG22 | 1.96                     | 0.65              |
| 39:DQ:18:LYS:H    | 39:DQ:98:LYS:HE2   | 1.60                     | 0.65              |
| 27:DA:143:G:O4'   | 46:DX:37:THR:HG21  | 1.96                     | 0.65              |
| 46:DX:26:TYR:CD2  | 46:DX:92:LEU:HD12  | 2.31                     | 0.65              |
| 47:DY:52:SER:O    | 47:DY:54:LYS:N     | 2.28                     | 0.65              |
| 3:AC:70:VAL:CG1   | 3:AC:72:LYS:H      | 2.09                     | 0.65              |
| 52:B3:29:ARG:HB2  | 52:B3:33:GLN:NE2   | 2.07                     | 0.65              |
| 57:B8:30:ARG:HA   | 57:B8:30:ARG:HE    | 1.61                     | 0.65              |
| 27:BA:1404:C:O2   | 27:BA:1404:C:H2'   | 1.96                     | 0.65              |
| 27:BA:1748:G:H8   | 27:BA:1748:G:H5'   | 1.61                     | 0.65              |
| 27:BA:816:C:H2'   | 27:BA:817:C:H6     | 1.61                     | 0.65              |
| 31:BE:57:LYS:CA   | 31:BE:59:VAL:HG12  | 2.26                     | 0.65              |
| 31:BE:86:PRO:C    | 31:BE:88:GLY:H     | 1.98                     | 0.65              |
| 32:BF:20:LEU:HB3  | 32:BF:23:ASP:CG    | 2.16                     | 0.65              |
| 32:BF:41:LEU:HD11 | 32:BF:184:TYR:CE1  | 2.30                     | 0.65              |
| 32:BF:45:ARG:NH1  | 32:BF:97:TYR:CE1   | 2.64                     | 0.65              |
| 32:BF:88:VAL:HG13 | 32:BF:89:VAL:O     | 1.95                     | 0.65              |
| 38:BP:6:LEU:HD12  | 38:BP:8:PRO:HG2    | 1.78                     | 0.65              |
| 42:BT:66:VAL:HA   | 42:BT:71:GLY:HA2   | 1.79                     | 0.65              |
| 46:BX:12:VAL:CG1  | 46:BX:17:ALA:HB1   | 2.25                     | 0.65              |
| 47:BY:26:LYS:HG2  | 47:BY:27:VAL:N     | 2.06                     | 0.65              |
| 1:CA:1220:G:O2'   | 1:CA:1221:G:H5'    | 1.96                     | 0.65              |
| 1:CA:677:U:H2'    | 1:CA:678:U:C6      | 2.32                     | 0.65              |
| 2:CB:51:LEU:HD23  | 2:CB:201:ILE:HD12  | 1.78                     | 0.65              |
| 3:CC:99:VAL:HG23  | 3:CC:99:VAL:O      | 1.96                     | 0.65              |
| 4:CD:134:ASP:OD2  | 4:CD:135:LEU:HD13  | 1.96                     | 0.65              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:CE:100:VAL:HG22   | 5:CE:118:ILE:HG22  | 1.79                     | 0.65              |
| 5:CE:29:GLY:HA2     | 5:CE:45:PHE:HE1    | 1.61                     | 0.65              |
| 24:CX:53:G:O2'      | 24:CX:54:U:H5'     | 1.95                     | 0.65              |
| 53:D4:44:CYS:SG     | 53:D4:64:LYS:HB2   | 2.37                     | 0.65              |
| 27:DA:1612:C:O3'    | 56:D7:5:TRP:HD1    | 1.79                     | 0.65              |
| 27:DA:1620:G:O4'    | 56:D7:1:MET:HA     | 1.96                     | 0.65              |
| 27:DA:203:C:H3'     | 27:DA:204:A:H5''   | 1.78                     | 0.65              |
| 31:DE:171:GLU:OE2   | 31:DE:173:VAL:HG23 | 1.96                     | 0.65              |
| 42:DT:88:ILE:CG2    | 42:DT:89:VAL:N     | 2.56                     | 0.65              |
| 44:DV:75:PHE:HD2    | 44:DV:82:ARG:HG3   | 1.61                     | 0.65              |
| 1:AA:324:G:C8       | 1:AA:324:G:H3'     | 2.31                     | 0.65              |
| 1:AA:618:C:H3'      | 1:AA:619:U:H5''    | 1.78                     | 0.65              |
| 1:AA:927:G:O2'      | 1:AA:928:G:H5'     | 1.96                     | 0.65              |
| 1:AA:544:G:OP1      | 4:AD:66:ARG:NH2    | 2.30                     | 0.65              |
| 5:AE:78:HIS:HD2     | 8:AH:104:ARG:CZ    | 2.09                     | 0.65              |
| 7:AG:137:LYS:O      | 7:AG:141:VAL:HG23  | 1.96                     | 0.65              |
| 24:AX:53:G:H2'      | 24:AX:54:U:H6      | 1.62                     | 0.65              |
| 49:B0:36:ILE:HD12   | 49:B0:37:LEU:N     | 2.11                     | 0.65              |
| 50:B1:19:GLN:HB2    | 50:B1:36:GLY:N     | 2.11                     | 0.65              |
| 51:B2:48:HIS:ND1    | 51:B2:49:LYS:N     | 2.45                     | 0.65              |
| 27:BA:1315:C:O2'    | 27:BA:1316:U:H5'   | 1.96                     | 0.65              |
| 27:BA:1695:G:N2     | 27:BA:1696:G:C8    | 2.65                     | 0.65              |
| 27:BA:2801(A):A:H4' | 27:BA:2802:G:C5'   | 2.20                     | 0.65              |
| 27:BA:644:A:H4'     | 27:BA:645:C:C5     | 2.30                     | 0.65              |
| 31:BE:200:GLU:HG2   | 31:BE:201:THR:N    | 2.12                     | 0.65              |
| 31:BE:3:GLY:O       | 31:BE:4:ILE:HB     | 1.95                     | 0.65              |
| 32:BF:21:ALA:O      | 32:BF:23:ASP:N     | 2.29                     | 0.65              |
| 33:BG:56:ALA:HA     | 33:BG:59:GLU:OE1   | 1.97                     | 0.65              |
| 35:BI:91:SER:CB     | 35:BI:119:PRO:HB2  | 2.26                     | 0.65              |
| 39:BQ:106:VAL:HG21  | 39:BQ:114:ALA:CB   | 2.26                     | 0.65              |
| 42:BT:32:TYR:CG     | 42:BT:81:PRO:HB2   | 2.30                     | 0.65              |
| 1:CA:179:A:C4       | 1:CA:180:U:C5      | 2.84                     | 0.65              |
| 1:CA:173:U:H1'      | 1:CA:197:A:C5      | 2.31                     | 0.65              |
| 1:CA:42:G:H2'       | 1:CA:43:C:C6       | 2.30                     | 0.65              |
| 1:CA:63:C:H5'       | 1:CA:64:G:OP2      | 1.96                     | 0.65              |
| 1:CA:568:G:N2       | 1:CA:883:C:C2      | 2.64                     | 0.65              |
| 5:CE:78:HIS:ND1     | 8:CH:107:LEU:CD1   | 2.60                     | 0.65              |
| 1:CA:376:G:H5''     | 16:CP:5:ARG:HG3    | 1.77                     | 0.65              |
| 18:CR:64:ARG:O      | 18:CR:65:ILE:C     | 2.33                     | 0.65              |
| 22:CV:1:A:H2'       | 22:CV:2:A:H5'      | 1.78                     | 0.65              |
| 27:DA:2230:G:C1'    | 50:D1:45:ASN:HB2   | 2.12                     | 0.65              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 55:D6:16:CYS:O      | 55:D6:17:LYS:HB2   | 1.95                     | 0.65              |
| 27:DA:1042:G:H5''   | 27:DA:1043:C:C6    | 2.31                     | 0.65              |
| 27:DA:1946:U:C2     | 27:DA:1947:C:C5    | 2.85                     | 0.65              |
| 31:DE:103:ASP:CG    | 31:DE:201:THR:HA   | 2.17                     | 0.65              |
| 41:DS:99:LYS:O      | 41:DS:101:LEU:N    | 2.29                     | 0.65              |
| 1:CA:1442(A):G:H22  | 42:DT:119:LYS:HB2  | 1.61                     | 0.65              |
| 45:DW:23:LEU:CD2    | 45:DW:39:THR:HG21  | 2.26                     | 0.65              |
| 47:DY:96:ILE:CG1    | 47:DY:99:CYS:HB2   | 2.26                     | 0.65              |
| 48:DZ:127:VAL:HG21  | 48:DZ:131:ASN:O    | 1.97                     | 0.65              |
| 48:DZ:27:MET:HE2    | 48:DZ:34:ARG:HB2   | 1.77                     | 0.65              |
| 1:AA:1019:C:O2'     | 1:AA:1020:U:H5'    | 1.97                     | 0.65              |
| 1:AA:415:A:H2'      | 1:AA:416:G:C8      | 2.32                     | 0.65              |
| 4:AD:149:ALA:O      | 4:AD:153:ARG:HG3   | 1.96                     | 0.65              |
| 4:AD:57:ARG:HD3     | 4:AD:205:GLU:CB    | 2.27                     | 0.65              |
| 4:AD:94:LEU:O       | 4:AD:97:LEU:HB2    | 1.97                     | 0.65              |
| 12:AL:82:ILE:CG2    | 12:AL:95:TYR:HB3   | 2.26                     | 0.65              |
| 49:B0:36:ILE:HD12   | 49:B0:36:ILE:C     | 2.17                     | 0.65              |
| 27:BA:271(A):A:H5'' | 27:BA:271(B):C:OP2 | 1.96                     | 0.65              |
| 27:BA:385:C:O2      | 27:BA:390:A:C2     | 2.49                     | 0.65              |
| 33:BG:2:PRO:O       | 33:BG:4:ASP:N      | 2.30                     | 0.65              |
| 46:BX:64:LYS:NZ     | 46:BX:73:ARG:NE    | 2.37                     | 0.65              |
| 47:BY:46:LYS:HG2    | 47:BY:47:LYS:HE3   | 1.78                     | 0.65              |
| 1:CA:1203:C:H2'     | 1:CA:1204:A:O4'    | 1.97                     | 0.65              |
| 1:CA:133:U:H1'      | 1:CA:230:G:N2      | 2.12                     | 0.65              |
| 1:CA:242:C:H2'      | 1:CA:243:A:H5'     | 1.79                     | 0.65              |
| 1:CA:964:A:H5''     | 1:CA:965:A:OP2     | 1.97                     | 0.65              |
| 2:CB:71:VAL:HB      | 2:CB:164:VAL:HG22  | 1.77                     | 0.65              |
| 4:CD:173:TRP:O      | 4:CD:174:LEU:HD23  | 1.95                     | 0.65              |
| 12:CL:4:ILE:HG22    | 12:CL:5:ASN:N      | 2.11                     | 0.65              |
| 19:CS:36:ARG:HA     | 19:CS:71:LEU:HB2   | 1.77                     | 0.65              |
| 54:D5:42:PRO:O      | 54:D5:43:HIS:HB2   | 1.97                     | 0.65              |
| 27:DA:1024:G:C3'    | 27:DA:1025:G:H5''  | 2.27                     | 0.65              |
| 27:DA:222:A:N6      | 27:DA:232:G:H1'    | 2.11                     | 0.65              |
| 27:DA:2236:C:C2'    | 27:DA:2237:G:H5'   | 2.27                     | 0.65              |
| 27:DA:2261:C:O2'    | 27:DA:2262:U:H5'   | 1.96                     | 0.65              |
| 27:DA:319:C:O2'     | 27:DA:320:A:H5'    | 1.96                     | 0.65              |
| 29:DC:66:HIS:ND1    | 29:DC:68:LEU:HG    | 2.12                     | 0.65              |
| 27:DA:1803:A:O2'    | 30:DD:259:THR:HG21 | 1.96                     | 0.65              |
| 32:DF:184:TYR:O     | 32:DF:188:ARG:HB2  | 1.96                     | 0.65              |
| 34:DH:149:ARG:HH21  | 34:DH:154:PRO:HG2  | 1.60                     | 0.65              |
| 36:DN:28:THR:HG23   | 36:DN:29:LYS:N     | 2.11                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:DO:101:PRO:HD2 | 42:DT:70:VAL:HG23  | 1.78                     | 0.65              |
| 39:DQ:81:VAL:CG2  | 39:DQ:82:ARG:N     | 2.60                     | 0.65              |
| 39:DQ:42:ILE:HD13 | 39:DQ:97:VAL:CG2   | 2.26                     | 0.65              |
| 40:DR:46:GLY:HA2  | 40:DR:49:ASP:HB2   | 1.78                     | 0.65              |
| 2:AB:238:LEU:O    | 2:AB:238:LEU:HG    | 1.97                     | 0.65              |
| 7:AG:140:ASP:HA   | 7:AG:143:ARG:NH1   | 2.11                     | 0.65              |
| 15:AO:3:ILE:HG22  | 15:AO:38:ARG:CZ    | 2.26                     | 0.65              |
| 27:BA:1504:C:H2'  | 27:BA:1505:C:H5''  | 1.79                     | 0.65              |
| 27:BA:1643:G:H21  | 27:BA:1644:C:H1'   | 1.61                     | 0.65              |
| 27:BA:2455:G:H2'  | 27:BA:2456:C:C6    | 2.31                     | 0.65              |
| 28:BB:8:U:H5'     | 28:BB:8:U:H6       | 1.60                     | 0.65              |
| 28:BB:94:C:C2'    | 28:BB:95:C:H5'     | 2.27                     | 0.65              |
| 30:BD:210:GLY:O   | 30:BD:211:ARG:HB2  | 1.96                     | 0.65              |
| 27:BA:1655:A:H4'  | 31:BE:115:GLY:H    | 1.62                     | 0.65              |
| 34:BH:147:ASN:O   | 34:BH:150:ALA:HB3  | 1.96                     | 0.65              |
| 37:BO:35:VAL:HG23 | 37:BO:65:THR:HG23  | 1.78                     | 0.65              |
| 42:BT:27:THR:OG1  | 42:BT:28:VAL:N     | 2.30                     | 0.65              |
| 42:BT:83:ILE:HG13 | 42:BT:84:GLN:H     | 1.60                     | 0.65              |
| 45:BW:45:TYR:O    | 45:BW:48:ALA:HB3   | 1.97                     | 0.65              |
| 47:BY:97:ARG:O    | 47:BY:97:ARG:HG3   | 1.97                     | 0.65              |
| 1:CA:1246:C:H2'   | 1:CA:1247:U:C6     | 2.31                     | 0.65              |
| 1:CA:339:C:H2'    | 1:CA:340:U:C6      | 2.32                     | 0.65              |
| 1:CA:413:G:N2     | 1:CA:428:G:O2'     | 2.27                     | 0.65              |
| 2:CB:207:ALA:O    | 2:CB:209:ARG:N     | 2.25                     | 0.65              |
| 3:CC:112:SER:HB3  | 3:CC:115:LEU:HD12  | 1.79                     | 0.65              |
| 12:CL:23:ALA:C    | 12:CL:24:LEU:HD22  | 2.16                     | 0.65              |
| 14:CN:26:ARG:CD   | 14:CN:43:CYS:SG    | 2.85                     | 0.65              |
| 15:CO:37:ASN:N    | 15:CO:37:ASN:HD22  | 1.95                     | 0.65              |
| 19:CS:18:LYS:HG2  | 19:CS:31:ILE:HD12  | 1.78                     | 0.65              |
| 38:DP:50:ARG:HB3  | 57:D8:59:LYS:HD3   | 1.77                     | 0.65              |
| 27:DA:1340:U:O2'  | 27:DA:1341:U:OP1   | 2.13                     | 0.65              |
| 27:DA:1299:G:H2'  | 27:DA:1639:U:O4    | 1.96                     | 0.65              |
| 27:DA:740:U:H2'   | 27:DA:741:G:H8     | 1.62                     | 0.65              |
| 28:DB:24:G:H4'    | 28:DB:25:A:H5'     | 1.79                     | 0.65              |
| 30:DD:181:GLU:HA  | 30:DD:272:ALA:CB   | 2.26                     | 0.65              |
| 30:DD:33:LEU:O    | 30:DD:34:VAL:HG12  | 1.95                     | 0.65              |
| 35:DI:77:LEU:HD22 | 35:DI:140:LEU:HD11 | 1.78                     | 0.65              |
| 38:DP:144:GLU:N   | 38:DP:145:PRO:HD3  | 2.08                     | 0.65              |
| 38:DP:50:ARG:HB3  | 57:D8:59:LYS:HD2   | 1.78                     | 0.65              |
| 42:DT:51:ARG:O    | 42:DT:61:PHE:HA    | 1.96                     | 0.65              |
| 48:DZ:93:GLU:O    | 48:DZ:129:PRO:HD3  | 1.96                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:101:A:O2'    | 1:AA:102:G:H5'     | 1.96                     | 0.65              |
| 1:AA:109:A:H4'    | 1:AA:110:C:OP2     | 1.93                     | 0.65              |
| 1:AA:253:U:H6     | 1:AA:253:U:H5'     | 1.61                     | 0.65              |
| 1:AA:451:A:H4'    | 1:AA:452:A:O5'     | 1.95                     | 0.65              |
| 3:AC:31:HIS:CD2   | 3:AC:31:HIS:H      | 2.13                     | 0.65              |
| 7:AG:146:GLU:HA   | 7:AG:149:ARG:HB2   | 1.78                     | 0.65              |
| 13:AM:5:ALA:CB    | 13:AM:66:LEU:HD22  | 2.27                     | 0.65              |
| 1:AA:1014:A:H4'   | 19:AS:14:HIS:CD2   | 2.32                     | 0.65              |
| 50:B1:58:ILE:HG12 | 50:B1:58:ILE:O     | 1.97                     | 0.65              |
| 27:BA:572:A:C2    | 27:BA:573:G:H1'    | 2.30                     | 0.65              |
| 30:BD:77:ALA:HB2  | 30:BD:97:TYR:HA    | 1.79                     | 0.65              |
| 27:BA:2810:A:H2'  | 31:BE:61:ARG:NH2   | 2.12                     | 0.65              |
| 31:BE:77:ILE:CG2  | 31:BE:78:LEU:H     | 1.96                     | 0.65              |
| 32:BF:52:LYS:HD3  | 32:BF:57:VAL:HA    | 1.76                     | 0.65              |
| 33:BG:35:GLU:OE1  | 33:BG:160:VAL:HG12 | 1.97                     | 0.65              |
| 33:BG:60:LEU:O    | 33:BG:64:THR:HG22  | 1.95                     | 0.65              |
| 35:BI:127:VAL:O   | 35:BI:128:LEU:HD23 | 1.96                     | 0.65              |
| 38:BP:89:ALA:HA   | 38:BP:121:LYS:HD3  | 1.77                     | 0.65              |
| 38:BP:17:LYS:HG2  | 38:BP:19:VAL:HG23  | 1.79                     | 0.65              |
| 27:BA:1754:C:P    | 42:BT:96:ARG:NH1   | 2.69                     | 0.65              |
| 43:BU:59:ARG:O    | 43:BU:60:LEU:C     | 2.35                     | 0.65              |
| 1:CA:1053:G:C6    | 1:CA:1199:U:H2'    | 2.30                     | 0.65              |
| 1:CA:1123:A:N3    | 10:CJ:38:ILE:HG22  | 2.12                     | 0.65              |
| 1:CA:955:U:O2'    | 1:CA:956:U:H5'     | 1.96                     | 0.65              |
| 5:CE:126:ARG:HH11 | 5:CE:126:ARG:HG3   | 1.62                     | 0.65              |
| 1:CA:1371:G:O3'   | 9:CI:69:GLY:HA3    | 1.97                     | 0.65              |
| 15:CO:10:LYS:HD2  | 15:CO:11:VAL:N     | 2.11                     | 0.65              |
| 27:DA:1017:G:C2'  | 27:DA:1018:C:H5'   | 2.26                     | 0.65              |
| 27:DA:1164:G:H2'  | 27:DA:1165:U:C6    | 2.32                     | 0.65              |
| 27:DA:1582:C:O2'  | 27:DA:1586:A:C8    | 2.47                     | 0.65              |
| 27:DA:2206:G:C2   | 27:DA:2207:G:H5'   | 2.32                     | 0.65              |
| 27:DA:2593:U:H2'  | 27:DA:2594:C:C5    | 2.31                     | 0.65              |
| 30:DD:43:ARG:NH1  | 30:DD:44:ASN:HD21  | 1.90                     | 0.65              |
| 38:DP:49:ARG:HD2  | 57:D8:58:ILE:CG2   | 2.26                     | 0.65              |
| 27:DA:910:A:H62   | 39:DQ:12:GLN:HA    | 1.60                     | 0.65              |
| 44:DV:76:LYS:HB2  | 44:DV:81:TYR:HB3   | 1.78                     | 0.65              |
| 45:DW:68:ARG:C    | 45:DW:110:LYS:HD3  | 2.16                     | 0.65              |
| 47:DY:27:VAL:CG1  | 47:DY:28:LYS:H     | 2.10                     | 0.65              |
| 1:AA:346:G:H5''   | 42:BT:41:ARG:NE    | 2.11                     | 0.65              |
| 1:AA:471:G:H2'    | 1:AA:472:A:C8      | 2.32                     | 0.65              |
| 1:AA:892:A:H2'    | 1:AA:893:C:C6      | 2.31                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:16:HIS:HB3    | 2:AB:210:SER:OG    | 1.96                     | 0.65              |
| 9:AI:16:ARG:O      | 9:AI:63:ILE:HG23   | 1.97                     | 0.65              |
| 12:AL:114:ARG:HH22 | 12:AL:121:LYS:HD3  | 1.62                     | 0.65              |
| 17:AQ:22:LEU:HD13  | 17:AQ:41:LYS:HG2   | 1.79                     | 0.65              |
| 58:B9:19:ARG:HG3   | 58:B9:24:TYR:CE1   | 2.32                     | 0.65              |
| 27:BA:1345:C:H2'   | 27:BA:1346:G:H8    | 1.61                     | 0.65              |
| 27:BA:2290:G:C8    | 27:BA:2290:G:H5'   | 2.30                     | 0.65              |
| 27:BA:248:G:N7     | 27:BA:250:G:N3     | 2.44                     | 0.65              |
| 27:BA:66:C:O2'     | 27:BA:67:U:H5'     | 1.95                     | 0.65              |
| 27:BA:89:G:H3'     | 27:BA:90:U:H5''    | 1.79                     | 0.65              |
| 29:BC:184:LYS:C    | 29:BC:186:ALA:H    | 1.99                     | 0.65              |
| 30:BD:68:LYS:NZ    | 30:BD:70:TRP:NE1   | 2.41                     | 0.65              |
| 34:BH:28:GLY:HA3   | 34:BH:79:VAL:HB    | 1.78                     | 0.65              |
| 35:BI:92:VAL:HG11  | 35:BI:120:ILE:HD12 | 1.79                     | 0.65              |
| 35:BI:114:LEU:HA   | 35:BI:130:TYR:HD1  | 1.60                     | 0.65              |
| 35:BI:72:LEU:O     | 35:BI:138:ILE:HD13 | 1.97                     | 0.65              |
| 46:BX:57:LEU:HD22  | 46:BX:57:LEU:O     | 1.97                     | 0.65              |
| 1:CA:1390:U:H2'    | 1:CA:1391:U:H6     | 1.59                     | 0.65              |
| 1:CA:1407:C:O2     | 27:DA:1912:A:H2    | 1.80                     | 0.65              |
| 1:CA:574:A:H5''    | 1:CA:575:G:OP2     | 1.97                     | 0.65              |
| 3:CC:47:LEU:CD2    | 3:CC:68:VAL:HG11   | 2.27                     | 0.65              |
| 4:CD:67:ILE:CD1    | 4:CD:196:LEU:HD23  | 2.26                     | 0.65              |
| 6:CF:3:ARG:HB3     | 6:CF:93:SER:HB2    | 1.79                     | 0.65              |
| 1:CA:1380:U:C5     | 7:CG:3:ARG:HG3     | 2.30                     | 0.65              |
| 14:CN:23:ARG:CZ    | 14:CN:30:ALA:HB2   | 2.27                     | 0.65              |
| 17:CQ:33:GLY:O     | 17:CQ:34:LYS:O     | 2.15                     | 0.65              |
| 55:D6:8:LYS:O      | 55:D6:9:LEU:HB2    | 1.97                     | 0.65              |
| 56:D7:24:THR:HG23  | 56:D7:27:GLY:HA3   | 1.78                     | 0.65              |
| 56:D7:27:GLY:O     | 56:D7:30:VAL:HG23  | 1.97                     | 0.65              |
| 57:D8:34:TRP:O     | 57:D8:35:GLN:HB2   | 1.95                     | 0.65              |
| 27:DA:1991:U:H2'   | 27:DA:1992:G:H5'   | 1.78                     | 0.65              |
| 27:DA:2024:G:H2'   | 27:DA:2025:C:O4'   | 1.96                     | 0.65              |
| 27:DA:363(E):U:H3' | 27:DA:363(F):A:O4' | 1.95                     | 0.65              |
| 27:DA:459:U:H2'    | 27:DA:460:A:C8     | 2.31                     | 0.65              |
| 27:DA:918:A:H3'    | 27:DA:919:G:H8     | 1.62                     | 0.65              |
| 30:DD:35:LYS:HZ1   | 30:DD:104:TYR:N    | 1.94                     | 0.65              |
| 36:DN:36:GLY:O     | 36:DN:38:HIS:N     | 2.30                     | 0.65              |
| 38:DP:101:VAL:CG1  | 38:DP:106:LEU:HD23 | 2.26                     | 0.65              |
| 41:DS:97:ARG:NH2   | 41:DS:98:VAL:CA    | 2.59                     | 0.65              |
| 42:DT:23:ARG:HH21  | 42:DT:120:ARG:HD3  | 1.62                     | 0.65              |
| 43:DU:50:ARG:NH2   | 44:DV:72:VAL:HG12  | 2.11                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:DW:40:ASN:O    | 45:DW:41:LYS:HG2  | 1.97                     | 0.65              |
| 45:DW:84:ARG:HG3  | 45:DW:98:LYS:HZ3  | 1.61                     | 0.65              |
| 1:AA:1060:C:C5    | 3:AC:2:GLY:HA2    | 2.32                     | 0.65              |
| 1:AA:279:A:H3'    | 17:AQ:95:TYR:OH   | 1.96                     | 0.65              |
| 13:AM:22:ILE:CG2  | 13:AM:25:ILE:HD13 | 2.27                     | 0.65              |
| 18:AR:57:GLY:C    | 18:AR:58:LEU:HD12 | 2.17                     | 0.65              |
| 19:AS:15:LEU:HD12 | 19:AS:31:ILE:HD11 | 1.79                     | 0.65              |
| 51:B2:48:HIS:HA   | 51:B2:51:ARG:HG2  | 1.77                     | 0.65              |
| 55:B6:29:ASN:CG   | 55:B6:30:THR:N    | 2.48                     | 0.65              |
| 27:BA:2443:C:H2'  | 27:BA:2444:G:C8   | 2.30                     | 0.65              |
| 27:BA:382:G:H2'   | 27:BA:383:U:H5'   | 1.78                     | 0.65              |
| 41:BS:87:PHE:O    | 41:BS:88:ASP:HB2  | 1.96                     | 0.65              |
| 43:BU:69:CYS:O    | 43:BU:74:LEU:HD12 | 1.96                     | 0.65              |
| 44:BV:99:ILE:N    | 44:BV:99:ILE:HD13 | 2.12                     | 0.65              |
| 1:CA:41:G:H1      | 1:CA:401:C:H42    | 1.44                     | 0.65              |
| 2:CB:236:TYR:HA   | 2:CB:239:VAL:HG23 | 1.77                     | 0.65              |
| 4:CD:76:ARG:O     | 4:CD:79:PHE:HB3   | 1.97                     | 0.65              |
| 9:CI:53:VAL:HG23  | 9:CI:54:ASP:H     | 1.60                     | 0.65              |
| 10:CJ:47:PHE:HB2  | 14:CN:34:TYR:HE2  | 1.62                     | 0.65              |
| 53:D4:61:VAL:HG13 | 53:D4:65:CYS:HB2  | 1.79                     | 0.65              |
| 54:D5:25:LEU:HD22 | 54:D5:26:THR:N    | 2.11                     | 0.65              |
| 27:DA:1388:G:O2'  | 27:DA:1389:G:H5'  | 1.97                     | 0.65              |
| 27:DA:1819:A:H5'' | 30:DD:158:ALA:CB  | 2.27                     | 0.65              |
| 27:DA:2394:C:H2'  | 27:DA:2395:C:H5'  | 1.78                     | 0.65              |
| 27:DA:2401:U:H2'  | 27:DA:2402:C:H5'' | 1.78                     | 0.65              |
| 27:DA:407:G:H2'   | 27:DA:408:G:C8    | 2.32                     | 0.65              |
| 27:DA:507:A:H4'   | 27:DA:509:C:C6    | 2.31                     | 0.65              |
| 28:DB:28:C:H2'    | 28:DB:29:A:C8     | 2.32                     | 0.65              |
| 28:DB:92:C:H2'    | 28:DB:93:G:H8     | 1.61                     | 0.65              |
| 47:DY:49:VAL:O    | 47:DY:50:ARG:HB2  | 1.97                     | 0.65              |
| 1:AA:1238:A:C2    | 1:AA:1241:G:H1'   | 2.32                     | 0.65              |
| 1:AA:1397:C:H3'   | 1:AA:1398:A:C5'   | 2.24                     | 0.65              |
| 1:AA:864:A:H2'    | 1:AA:865:A:C8     | 2.32                     | 0.65              |
| 7:AG:60:LYS:NZ    | 7:AG:63:LYS:HB3   | 2.12                     | 0.65              |
| 10:AJ:34:VAL:HG13 | 10:AJ:73:ASP:O    | 1.97                     | 0.65              |
| 13:AM:8:GLU:OE2   | 13:AM:22:ILE:HA   | 1.96                     | 0.65              |
| 35:BI:27:ARG:HD2  | 50:B1:71:TYR:CD1  | 2.32                     | 0.65              |
| 51:B2:53:LEU:HD13 | 51:B2:57:ILE:HD11 | 1.78                     | 0.65              |
| 27:BA:1262:A:N3   | 54:B5:10:LYS:NZ   | 2.45                     | 0.65              |
| 27:BA:1931:U:H6   | 27:BA:1931:U:H5'  | 1.62                     | 0.65              |
| 27:BA:2065:C:H2'  | 27:BA:2066:C:C6   | 2.30                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2230:G:O3'  | 50:B1:43:TYR:HB2   | 1.97                     | 0.65              |
| 27:BA:2239:G:H2'  | 27:BA:2240:C:H6    | 1.62                     | 0.65              |
| 27:BA:2564:A:C2   | 27:BA:2647:U:H4'   | 2.32                     | 0.65              |
| 32:BF:67:GLN:CG   | 32:BF:67:GLN:O     | 2.33                     | 0.65              |
| 34:BH:20:ALA:HB1  | 34:BH:21:PRO:CD    | 2.27                     | 0.65              |
| 35:BI:73:GLU:HB2  | 35:BI:136:VAL:HG23 | 1.78                     | 0.65              |
| 37:BO:66:LYS:H    | 37:BO:82:ASN:HD21  | 1.45                     | 0.65              |
| 41:BS:82:ILE:HD13 | 41:BS:82:ILE:N     | 2.09                     | 0.65              |
| 1:CA:1520:G:O2'   | 1:CA:1521:G:H5'    | 1.97                     | 0.65              |
| 1:CA:963:G:H21    | 10:CJ:55:LYS:HZ2   | 1.44                     | 0.65              |
| 2:CB:164:VAL:O    | 2:CB:186:ALA:HB1   | 1.97                     | 0.65              |
| 2:CB:194:PRO:O    | 2:CB:196:LEU:N     | 2.29                     | 0.65              |
| 19:CS:9:VAL:HB    | 19:CS:11:VAL:HG12  | 1.79                     | 0.65              |
| 54:D5:31:VAL:HB   | 54:D5:32:PRO:CD    | 2.27                     | 0.65              |
| 27:DA:1422:G:H1'  | 27:DA:1496:A:H62   | 1.62                     | 0.65              |
| 27:DA:1665:A:H2'  | 27:DA:1666:G:O4'   | 1.97                     | 0.65              |
| 27:DA:2564:A:OP1  | 27:DA:2648:C:H4'   | 1.96                     | 0.65              |
| 30:DD:43:ARG:HD2  | 30:DD:44:ASN:OD1   | 1.96                     | 0.65              |
| 27:DA:1568:G:OP1  | 30:DD:61:LEU:HB2   | 1.96                     | 0.65              |
| 31:DE:11:MET:HB2  | 31:DE:23:VAL:O     | 1.97                     | 0.65              |
| 32:DF:38:ARG:HH21 | 32:DF:99:TYR:HE1   | 1.45                     | 0.65              |
| 43:DU:65:ILE:HD11 | 43:DU:96:ALA:CB    | 2.27                     | 0.65              |
| 43:DU:84:LYS:HD2  | 43:DU:89:GLU:HB3   | 1.78                     | 0.65              |
| 44:DV:38:LEU:HD13 | 44:DV:55:ALA:HB1   | 1.78                     | 0.65              |
| 1:AA:123:C:OP1    | 1:AA:312:C:H5'     | 1.97                     | 0.65              |
| 1:AA:454:C:H2'    | 1:AA:455:C:C6      | 2.32                     | 0.65              |
| 1:AA:72:C:H2'     | 1:AA:73:G:C8       | 2.31                     | 0.65              |
| 4:AD:101:LEU:O    | 4:AD:104:VAL:HG12  | 1.97                     | 0.65              |
| 1:AA:676:A:C1'    | 11:AK:115:PRO:HB3  | 2.22                     | 0.65              |
| 13:AM:68:GLY:CA   | 13:AM:71:ARG:HH21  | 2.09                     | 0.65              |
| 18:AR:55:ARG:HG3  | 18:AR:55:ARG:HH11  | 1.62                     | 0.65              |
| 27:BA:1013:C:O2'  | 27:BA:1014:U:H5'   | 1.96                     | 0.65              |
| 27:BA:1175:U:H2'  | 27:BA:1175:U:O2    | 1.97                     | 0.65              |
| 27:BA:425:G:H2'   | 27:BA:426:C:H6     | 1.62                     | 0.65              |
| 29:BC:83:ILE:HA   | 29:BC:94:VAL:HG21  | 1.79                     | 0.65              |
| 30:BD:31:LYS:CG   | 30:BD:33:LEU:HD13  | 2.25                     | 0.65              |
| 32:BF:25:PRO:HG3  | 32:BF:119:ARG:HB2  | 1.77                     | 0.65              |
| 33:BG:113:ARG:O   | 33:BG:140:ILE:HG23 | 1.97                     | 0.65              |
| 33:BG:2:PRO:HG2   | 53:B4:51:TYR:CE2   | 2.32                     | 0.65              |
| 35:BI:115:ALA:HB3 | 35:BI:129:THR:N    | 2.11                     | 0.65              |
| 36:BN:1:MET:O     | 36:BN:2:LYS:HG3    | 1.97                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BP:88:LEU:O    | 38:BP:90:ARG:N    | 2.30                     | 0.65              |
| 40:BR:101:ALA:O   | 40:BR:102:GLU:CB  | 2.44                     | 0.65              |
| 37:BO:77:ILE:HD11 | 42:BT:72:VAL:HG11 | 1.79                     | 0.65              |
| 44:BV:2:PHE:HD2   | 44:BV:42:GLY:HA2  | 1.62                     | 0.65              |
| 46:BX:12:VAL:HG11 | 46:BX:17:ALA:HB1  | 1.79                     | 0.65              |
| 3:CC:52:LEU:CD2   | 3:CC:52:LEU:H     | 2.10                     | 0.65              |
| 10:CJ:8:LEU:HD12  | 10:CJ:20:ALA:HB2  | 1.78                     | 0.65              |
| 15:CO:75:PRO:O    | 15:CO:78:TYR:HB3  | 1.97                     | 0.65              |
| 23:CW:63:C:H2'    | 23:CW:64:G:H8     | 1.61                     | 0.65              |
| 49:D0:5:LYS:HB3   | 49:D0:5:LYS:NZ    | 2.11                     | 0.65              |
| 51:D2:3:LEU:HD22  | 51:D2:7:ARG:HH12  | 1.60                     | 0.65              |
| 27:DA:107:C:H2'   | 27:DA:108:U:H6    | 1.62                     | 0.65              |
| 27:DA:1655:A:H3'  | 27:DA:1656:C:C6   | 2.31                     | 0.65              |
| 27:DA:1887:C:H3'  | 27:DA:1888:G:H5'' | 1.77                     | 0.65              |
| 27:DA:2406:U:N3   | 38:DP:72:PRO:HB2  | 2.12                     | 0.65              |
| 27:DA:2648:C:H2'  | 27:DA:2649:U:C6   | 2.32                     | 0.65              |
| 27:DA:2808:U:C2'  | 27:DA:2809:A:H5'  | 2.26                     | 0.65              |
| 43:DU:42:ALA:O    | 43:DU:44:ASN:N    | 2.30                     | 0.65              |
| 44:DV:38:LEU:HD12 | 44:DV:56:SER:CA   | 2.26                     | 0.65              |
| 44:DV:95:LEU:HD13 | 44:DV:97:LYS:NZ   | 2.12                     | 0.65              |
| 1:AA:1209:C:O2'   | 1:AA:1210:C:H5'   | 1.97                     | 0.64              |
| 1:AA:419:C:H2'    | 1:AA:420:U:H5'    | 1.79                     | 0.64              |
| 1:AA:942:G:N2     | 1:AA:943:U:C2     | 2.64                     | 0.64              |
| 8:AH:108:GLY:HA3  | 8:AH:138:TRP:HB3  | 1.79                     | 0.64              |
| 9:AI:21:PRO:HA    | 9:AI:58:HIS:O     | 1.96                     | 0.64              |
| 27:BA:372:G:H3'   | 50:B1:66:HIS:CE1  | 2.33                     | 0.64              |
| 54:B5:16:ARG:NH1  | 54:B5:17:ASP:CG   | 2.51                     | 0.64              |
| 54:B5:41:PRO:HG2  | 54:B5:44:THR:CG2  | 2.27                     | 0.64              |
| 27:BA:1517:G:H2'  | 27:BA:1518:U:O4'  | 1.97                     | 0.64              |
| 27:BA:2331:G:O2'  | 49:B0:43:THR:HG22 | 1.96                     | 0.64              |
| 27:BA:2357:U:H2'  | 27:BA:2358:G:H5'' | 1.79                     | 0.64              |
| 27:BA:754:C:H6    | 27:BA:754:C:H5'   | 1.62                     | 0.64              |
| 27:BA:2580:U:H4'  | 31:BE:131:ALA:H   | 1.62                     | 0.64              |
| 36:BN:119:ARG:O   | 36:BN:120:LEU:HB2 | 1.97                     | 0.64              |
| 38:BP:88:LEU:C    | 38:BP:90:ARG:H    | 1.98                     | 0.64              |
| 48:BZ:29:ASN:O    | 48:BZ:30:ARG:HB3  | 1.96                     | 0.64              |
| 1:CA:1160:G:O2'   | 1:CA:1161:C:H5'   | 1.97                     | 0.64              |
| 1:CA:261:U:O2     | 1:CA:263:A:H8     | 1.81                     | 0.64              |
| 2:CB:189:ASP:HB3  | 2:CB:203:GLY:O    | 1.97                     | 0.64              |
| 1:CA:1152:A:H5''  | 10:CJ:13:HIS:HB2  | 1.79                     | 0.64              |
| 56:D7:9:ARG:HB3   | 56:D7:48:LYS:HZ3  | 1.60                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1747:G:H2'   | 27:DA:1747(A):G:C8 | 2.26                     | 0.64              |
| 27:DA:2373:G:O2'   | 27:DA:2374:C:H5'   | 1.97                     | 0.64              |
| 27:DA:2605:U:H2'   | 27:DA:2606:C:C6    | 2.32                     | 0.64              |
| 27:DA:377:C:H2'    | 27:DA:378:C:H6     | 1.60                     | 0.64              |
| 27:DA:679:C:O2'    | 27:DA:680:G:H5'    | 1.96                     | 0.64              |
| 27:DA:920:G:O2'    | 27:DA:921:G:H5'    | 1.96                     | 0.64              |
| 30:DD:168:ARG:N    | 30:DD:168:ARG:HD3  | 2.11                     | 0.64              |
| 30:DD:186:HIS:HD2  | 30:DD:188:GLU:HB2  | 1.62                     | 0.64              |
| 31:DE:131:ALA:HB3  | 31:DE:134:ILE:HD11 | 1.79                     | 0.64              |
| 36:DN:82:LEU:C     | 36:DN:82:LEU:HD12  | 2.18                     | 0.64              |
| 42:DT:19:LEU:HD12  | 42:DT:19:LEU:H     | 1.62                     | 0.64              |
| 42:DT:8:LYS:O      | 42:DT:11:GLU:OE1   | 2.15                     | 0.64              |
| 44:DV:18:LEU:HD22  | 44:DV:19:LYS:N     | 2.05                     | 0.64              |
| 48:DZ:150:HIS:HB3  | 48:DZ:169:THR:HA   | 1.79                     | 0.64              |
| 7:AG:23:VAL:HG12   | 7:AG:27:ILE:HD11   | 1.79                     | 0.64              |
| 12:AL:43:LYS:HG2   | 12:AL:44:LYS:N     | 2.12                     | 0.64              |
| 13:AM:75:ALA:O     | 13:AM:79:LYS:HG3   | 1.96                     | 0.64              |
| 15:AO:30:ALA:HB2   | 15:AO:85:LEU:HD11  | 1.79                     | 0.64              |
| 23:AW:70:C:O2'     | 23:AW:71:A:H5'     | 1.96                     | 0.64              |
| 25:AY:65:U:H2'     | 25:AY:66:A:H8      | 1.62                     | 0.64              |
| 50:B1:18:ILE:C     | 50:B1:19:GLN:HE21  | 2.00                     | 0.64              |
| 57:B8:4:MET:HB3    | 57:B8:61:LEU:HD22  | 1.79                     | 0.64              |
| 27:BA:1275:A:H4'   | 27:BA:1276:A:OP1   | 1.96                     | 0.64              |
| 27:BA:1337:G:H2'   | 27:BA:1338:G:H8    | 1.59                     | 0.64              |
| 27:BA:2869:G:H2'   | 27:BA:2870:C:H6    | 1.62                     | 0.64              |
| 31:BE:39:PRO:O     | 31:BE:43:GLY:HA2   | 1.98                     | 0.64              |
| 32:BF:51:THR:HG21  | 32:BF:92:PRO:HD2   | 1.80                     | 0.64              |
| 33:BG:101:ILE:HD13 | 33:BG:102:PHE:N    | 2.12                     | 0.64              |
| 33:BG:47:LYS:HD3   | 33:BG:82:LEU:HD12  | 1.79                     | 0.64              |
| 34:BH:85:LYS:HZ2   | 34:BH:133:VAL:CB   | 2.09                     | 0.64              |
| 36:BN:17:ASP:HB2   | 36:BN:55:VAL:HG13  | 1.78                     | 0.64              |
| 43:BU:104:GLN:NE2  | 43:BU:105:VAL:N    | 2.46                     | 0.64              |
| 44:BV:46:VAL:HG22  | 44:BV:47:VAL:N     | 2.08                     | 0.64              |
| 1:CA:1200:C:O2'    | 1:CA:1201:A:OP2    | 2.06                     | 0.64              |
| 1:CA:14:U:H5'      | 1:CA:14:U:H6       | 1.62                     | 0.64              |
| 1:CA:815:A:O2'     | 1:CA:1527:C:H1'    | 1.97                     | 0.64              |
| 1:CA:628:G:O2'     | 1:CA:629:G:H5'     | 1.97                     | 0.64              |
| 2:CB:41:ILE:HG22   | 2:CB:41:ILE:O      | 1.97                     | 0.64              |
| 5:CE:48:ALA:HB1    | 5:CE:49:PRO:CD     | 2.27                     | 0.64              |
| 11:CK:79:SER:HB2   | 11:CK:106:LYS:CD   | 2.27                     | 0.64              |
| 13:CM:95:GLY:O     | 13:CM:96:LEU:CB    | 2.45                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:CQ:29:HIS:CD2   | 17:CQ:30:PRO:HD2   | 2.33                     | 0.64              |
| 19:CS:35:SER:O     | 19:CS:71:LEU:HD12  | 1.97                     | 0.64              |
| 13:CM:84:ILE:H     | 19:CS:66:MET:HE1   | 1.62                     | 0.64              |
| 52:D3:6:VAL:HG12   | 52:D3:56:VAL:HA    | 1.78                     | 0.64              |
| 56:D7:40:TRP:HB2   | 56:D7:41:ARG:NH2   | 2.12                     | 0.64              |
| 27:DA:1213:A:H2'   | 27:DA:1214:A:C8    | 2.32                     | 0.64              |
| 27:DA:1304:C:H42   | 27:DA:1624:G:H1    | 1.43                     | 0.64              |
| 27:DA:335:C:H5''   | 47:DY:73:ARG:NH2   | 2.12                     | 0.64              |
| 29:DC:168:THR:HA   | 29:DC:173:ALA:CB   | 2.28                     | 0.64              |
| 33:DG:46:ALA:C     | 33:DG:51:ARG:HG3   | 2.17                     | 0.64              |
| 36:DN:22:THR:HA    | 36:DN:60:ILE:HG22  | 1.79                     | 0.64              |
| 41:DS:21:THR:C     | 41:DS:23:ARG:H     | 2.01                     | 0.64              |
| 45:DW:88:ARG:HB2   | 45:DW:92:ARG:HB3   | 1.79                     | 0.64              |
| 1:AA:403:C:O2'     | 1:AA:404:U:H5'     | 1.95                     | 0.64              |
| 1:AA:812:C:OP1     | 1:AA:903:G:H1'     | 1.97                     | 0.64              |
| 5:AE:150:ARG:HA    | 5:AE:153:LYS:HE2   | 1.79                     | 0.64              |
| 17:AQ:54:GLY:HA3   | 17:AQ:82:MET:SD    | 2.37                     | 0.64              |
| 50:B1:19:GLN:CB    | 50:B1:35:THR:HG23  | 2.27                     | 0.64              |
| 51:B2:13:ALA:O     | 51:B2:16:LEU:HG    | 1.97                     | 0.64              |
| 52:B3:8:LEU:HD13   | 52:B3:31:LEU:HA    | 1.79                     | 0.64              |
| 27:BA:1363:C:O2'   | 27:BA:1364:G:H5'   | 1.97                     | 0.64              |
| 27:BA:1490:A:H2    | 30:BD:75:ILE:HG23  | 1.62                     | 0.64              |
| 27:BA:1888:G:N3    | 27:BA:1888:G:H5'   | 2.12                     | 0.64              |
| 27:BA:2862:G:H2'   | 27:BA:2863:C:H6    | 1.62                     | 0.64              |
| 27:BA:363(A):A:H5' | 27:BA:363(B):G:OP2 | 1.97                     | 0.64              |
| 27:BA:542:C:H2'    | 27:BA:543:C:OP1    | 1.97                     | 0.64              |
| 31:BE:49:LEU:HD12  | 31:BE:49:LEU:N     | 2.13                     | 0.64              |
| 31:BE:93:VAL:C     | 31:BE:95:ILE:H     | 2.01                     | 0.64              |
| 32:BF:143:ALA:HB1  | 32:BF:148:LEU:HB2  | 1.79                     | 0.64              |
| 32:BF:32:LEU:O     | 32:BF:32:LEU:HD23  | 1.98                     | 0.64              |
| 33:BG:125:PHE:CD2  | 33:BG:131:TYR:HB2  | 2.32                     | 0.64              |
| 33:BG:72:ARG:HD3   | 33:BG:86:MET:HA    | 1.80                     | 0.64              |
| 34:BH:94:TYR:C     | 34:BH:95:ARG:HG2   | 2.17                     | 0.64              |
| 37:BO:122:LEU:HA   | 42:BT:43:GLN:HE22  | 1.62                     | 0.64              |
| 48:BZ:123:ILE:HG12 | 48:BZ:124:LEU:N    | 2.10                     | 0.64              |
| 2:CB:131:PRO:HG2   | 2:CB:134:GLU:HB2   | 1.78                     | 0.64              |
| 4:CD:202:LEU:HD23  | 4:CD:205:GLU:OE2   | 1.97                     | 0.64              |
| 5:CE:76:ILE:CG1    | 5:CE:77:PRO:HD2    | 2.28                     | 0.64              |
| 50:D1:57:GLU:O     | 50:D1:58:ILE:HG12  | 1.96                     | 0.64              |
| 27:DA:1188:U:O2'   | 27:DA:1189:A:H5'   | 1.97                     | 0.64              |
| 27:DA:1301:A:H4'   | 27:DA:1302:A:OP1   | 1.96                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:142:A:H8    | 27:DA:1595:G:H21  | 1.38                     | 0.64              |
| 27:DA:1682:G:H2'  | 27:DA:1683:C:C6   | 2.33                     | 0.64              |
| 27:DA:1770:G:H2'  | 27:DA:1771:C:H6   | 1.63                     | 0.64              |
| 27:DA:1948:G:C4   | 27:DA:1959:G:N2   | 2.65                     | 0.64              |
| 27:DA:2512:C:H42  | 27:DA:2574:G:H1   | 1.44                     | 0.64              |
| 27:DA:527:C:H5''  | 27:DA:528:A:OP1   | 1.97                     | 0.64              |
| 27:DA:925:C:H2'   | 27:DA:926:A:H5''  | 1.79                     | 0.64              |
| 33:DG:60:LEU:HD12 | 33:DG:68:PRO:CG   | 2.27                     | 0.64              |
| 34:DH:38:SER:C    | 34:DH:40:GLU:H    | 2.00                     | 0.64              |
| 34:DH:43:VAL:HG11 | 34:DH:52:VAL:HA   | 1.77                     | 0.64              |
| 39:DQ:69:PHE:CD1  | 39:DQ:70:PRO:HD2  | 2.33                     | 0.64              |
| 39:DQ:43:THR:HG22 | 39:DQ:94:VAL:CG1  | 2.27                     | 0.64              |
| 42:DT:6:LEU:HD23  | 42:DT:6:LEU:O     | 1.97                     | 0.64              |
| 48:DZ:102:ARG:HD3 | 48:DZ:135:PHE:CE1 | 2.33                     | 0.64              |
| 1:AA:1064:G:H21   | 1:AA:1190:G:H2'   | 1.61                     | 0.64              |
| 1:AA:390:C:H4'    | 16:AP:28:ARG:HH21 | 1.61                     | 0.64              |
| 1:AA:445:G:O2'    | 1:AA:446:G:H5'    | 1.97                     | 0.64              |
| 8:AH:64:LYS:HG2   | 8:AH:79:VAL:HG21  | 1.79                     | 0.64              |
| 13:AM:78:ILE:HA   | 13:AM:81:LEU:HD13 | 1.78                     | 0.64              |
| 16:AP:57:ARG:HA   | 16:AP:60:LEU:HD12 | 1.79                     | 0.64              |
| 19:AS:6:LYS:HG2   | 19:AS:7:LYS:CE    | 2.26                     | 0.64              |
| 19:AS:6:LYS:CD    | 19:AS:7:LYS:HE3   | 2.27                     | 0.64              |
| 23:AW:74:C:H2'    | 23:AW:75:A:C8     | 2.32                     | 0.64              |
| 53:B4:36:VAL:HB   | 53:B4:37:PRO:HD2  | 1.80                     | 0.64              |
| 27:BA:2481:G:O2'  | 27:BA:2482:G:P    | 2.55                     | 0.64              |
| 27:BA:380:U:H3    | 27:BA:394:A:N6    | 1.94                     | 0.64              |
| 27:BA:491:G:O2'   | 27:BA:492:A:H5'   | 1.97                     | 0.64              |
| 27:BA:624:C:H41   | 38:BP:107:LYS:NZ  | 1.96                     | 0.64              |
| 27:BA:686:G:N2    | 27:BA:788:A:H61   | 1.96                     | 0.64              |
| 30:BD:60:ARG:HD3  | 30:BD:86:PRO:HB2  | 1.79                     | 0.64              |
| 34:BH:70:THR:OG1  | 34:BH:71:LEU:N    | 2.28                     | 0.64              |
| 34:BH:92:ILE:O    | 34:BH:94:TYR:N    | 2.24                     | 0.64              |
| 35:BI:117:GLU:HG3 | 35:BI:118:LYS:H   | 1.62                     | 0.64              |
| 36:BN:95:PRO:O    | 36:BN:98:VAL:HG23 | 1.97                     | 0.64              |
| 39:BQ:140:ALA:O   | 48:BZ:52:ILE:HD13 | 1.96                     | 0.64              |
| 39:BQ:51:ARG:O    | 39:BQ:55:VAL:HG12 | 1.97                     | 0.64              |
| 41:BS:30:ARG:NH2  | 41:BS:62:LYS:HD2  | 2.10                     | 0.64              |
| 1:CA:501:C:H2'    | 1:CA:502:G:C8     | 2.32                     | 0.64              |
| 17:CQ:82:MET:HA   | 17:CQ:85:VAL:HG23 | 1.79                     | 0.64              |
| 49:D0:75:LEU:HD22 | 49:D0:78:TYR:OH   | 1.97                     | 0.64              |
| 52:D3:23:LEU:H    | 52:D3:23:LEU:HD12 | 1.63                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 54:D5:37:LYS:HG3   | 54:D5:38:ALA:H    | 1.62                     | 0.64              |
| 27:DA:1131:G:HO2'  | 27:DA:1132:A:H8   | 1.45                     | 0.64              |
| 27:DA:1515:G:H2'   | 27:DA:1516:C:C6   | 2.32                     | 0.64              |
| 27:DA:1568:G:H5''  | 30:DD:61:LEU:CD2  | 2.20                     | 0.64              |
| 27:DA:1743:C:H2'   | 27:DA:1744:C:O4'  | 1.97                     | 0.64              |
| 27:DA:212:G:O2'    | 27:DA:213:A:H5'   | 1.97                     | 0.64              |
| 27:DA:2330:G:H21   | 49:D0:42:GLY:HA2  | 1.61                     | 0.64              |
| 27:DA:2689:U:H5''  | 27:DA:2690:C:H5'  | 1.79                     | 0.64              |
| 27:DA:2897:U:H2'   | 27:DA:2897:U:O2   | 1.95                     | 0.64              |
| 31:DE:127:ASP:HA   | 31:DE:135:HIS:CE1 | 2.32                     | 0.64              |
| 31:DE:59:VAL:HG13  | 31:DE:60:ASN:N    | 2.12                     | 0.64              |
| 32:DF:159:GLY:O    | 32:DF:161:GLU:HG3 | 1.98                     | 0.64              |
| 33:DG:41:GLN:HG2   | 33:DG:155:MET:HB3 | 1.79                     | 0.64              |
| 39:DQ:85:LYS:HG3   | 49:D0:7:LEU:CD1   | 2.25                     | 0.64              |
| 45:DW:68:ARG:HB3   | 45:DW:110:LYS:HB2 | 1.78                     | 0.64              |
| 46:DX:12:VAL:HG12  | 46:DX:27:THR:CG2  | 2.27                     | 0.64              |
| 47:DY:27:VAL:HG12  | 47:DY:29:GLU:OE1  | 1.96                     | 0.64              |
| 4:AD:9:CYS:SG      | 4:AD:22:LYS:HD2   | 2.37                     | 0.64              |
| 5:AE:139:LEU:HA    | 5:AE:142:LEU:HD12 | 1.80                     | 0.64              |
| 5:AE:8:GLU:HA      | 5:AE:34:VAL:HA    | 1.79                     | 0.64              |
| 9:AI:4:TYR:H       | 9:AI:4:TYR:HD1    | 1.43                     | 0.64              |
| 11:AK:51:LYS:HB3   | 11:AK:51:LYS:NZ   | 2.13                     | 0.64              |
| 13:AM:89:GLY:O     | 13:AM:93:ARG:HD2  | 1.98                     | 0.64              |
| 16:AP:16:HIS:HE1   | 16:AP:42:ARG:HH21 | 1.43                     | 0.64              |
| 17:AQ:56:VAL:HG21  | 17:AQ:78:GLU:HG2  | 1.78                     | 0.64              |
| 6:AF:91:VAL:HG13   | 18:AR:72:ARG:NH2  | 2.13                     | 0.64              |
| 53:B4:41:ILE:HG12  | 53:B4:57:ILE:O    | 1.97                     | 0.64              |
| 55:B6:11:LEU:CD1   | 55:B6:51:GLU:HG2  | 2.28                     | 0.64              |
| 27:BA:1683:C:H2'   | 27:BA:1684:C:C6   | 2.33                     | 0.64              |
| 27:BA:2447:G:H4'   | 27:BA:2448:A:O5'  | 1.97                     | 0.64              |
| 31:BE:199:ARG:O    | 31:BE:200:GLU:O   | 2.15                     | 0.64              |
| 34:BH:113:VAL:HG21 | 34:BH:151:ILE:CG2 | 2.25                     | 0.64              |
| 34:BH:43:VAL:O     | 34:BH:43:VAL:HG23 | 1.98                     | 0.64              |
| 38:BP:48:PRO:O     | 38:BP:50:ARG:N    | 2.31                     | 0.64              |
| 39:BQ:56:ARG:HG2   | 39:BQ:56:ARG:HH11 | 1.62                     | 0.64              |
| 42:BT:28:VAL:HG21  | 42:BT:46:GLU:HG3  | 1.78                     | 0.64              |
| 46:BX:54:VAL:HG13  | 46:BX:81:VAL:HG13 | 1.80                     | 0.64              |
| 1:CA:1499:A:H1'    | 1:CA:1520:G:H5'   | 1.78                     | 0.64              |
| 5:CE:75:THR:OG1    | 5:CE:76:ILE:N     | 2.29                     | 0.64              |
| 10:CJ:40:LEU:HD21  | 10:CJ:69:ASN:HB3  | 1.79                     | 0.64              |
| 12:CL:14:LYS:HD3   | 12:CL:15:VAL:HG22 | 1.79                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:1041:C:H2'   | 27:DA:1042:G:C8   | 2.32                     | 0.64              |
| 27:DA:1237:A:H2    | 27:DA:1238:G:N3   | 1.95                     | 0.64              |
| 27:DA:1673:U:C2'   | 27:DA:1674:G:H5'  | 2.26                     | 0.64              |
| 27:DA:1799:G:H4'   | 27:DA:1800:C:O5'  | 1.95                     | 0.64              |
| 27:DA:2267:A:H3'   | 27:DA:2268:A:H5'' | 1.80                     | 0.64              |
| 27:DA:548:A:O2'    | 27:DA:549:G:H5'   | 1.98                     | 0.64              |
| 27:DA:704:G:H1'    | 27:DA:727:A:N6    | 2.12                     | 0.64              |
| 32:DF:128:ALA:O    | 32:DF:130:ALA:N   | 2.31                     | 0.64              |
| 27:DA:2667:C:H1'   | 34:DH:109:PHE:CD2 | 2.31                     | 0.64              |
| 37:DO:107:ARG:NH1  | 42:DT:35:LYS:HB2  | 2.12                     | 0.64              |
| 39:DQ:130:LYS:HG3  | 39:DQ:131:ILE:H   | 1.62                     | 0.64              |
| 41:DS:19:LYS:O     | 41:DS:20:ARG:NH1  | 2.28                     | 0.64              |
| 44:DV:5:VAL:HG23   | 44:DV:37:VAL:HG23 | 1.79                     | 0.64              |
| 1:AA:554:C:O2'     | 1:AA:555:C:H5'    | 1.97                     | 0.64              |
| 2:AB:194:PRO:HA    | 2:AB:200:ILE:HD13 | 1.79                     | 0.64              |
| 4:AD:128:VAL:C     | 4:AD:130:GLY:N    | 2.49                     | 0.64              |
| 12:AL:21:VAL:CG1   | 12:AL:23:ALA:HB2  | 2.28                     | 0.64              |
| 12:AL:43:LYS:CG    | 12:AL:44:LYS:H    | 2.10                     | 0.64              |
| 12:AL:75:GLN:O     | 12:AL:78:SER:HB2  | 1.98                     | 0.64              |
| 15:AO:5:LYS:HA     | 15:AO:8:LYS:HB3   | 1.79                     | 0.64              |
| 18:AR:44:LEU:HD22  | 18:AR:48:GLY:O    | 1.98                     | 0.64              |
| 27:BA:1826:G:H4'   | 30:BD:242:ARG:NH2 | 2.12                     | 0.64              |
| 27:BA:2113:U:H2'   | 27:BA:2114:A:C8   | 2.33                     | 0.64              |
| 27:BA:2223:G:H2'   | 27:BA:2224:G:H5'  | 1.80                     | 0.64              |
| 27:BA:2681:C:C5    | 27:BA:2725:A:N6   | 2.64                     | 0.64              |
| 27:BA:271(G):C:H2' | 27:BA:271(H):G:H8 | 1.63                     | 0.64              |
| 27:BA:582:G:H2'    | 27:BA:583:G:H8    | 1.62                     | 0.64              |
| 38:BP:16:ARG:O     | 38:BP:16:ARG:NH1  | 2.30                     | 0.64              |
| 41:BS:61:ASN:O     | 41:BS:62:LYS:HG2  | 1.98                     | 0.64              |
| 47:BY:90:LEU:CD1   | 47:BY:91:GLU:H    | 2.06                     | 0.64              |
| 48:BZ:107:PRO:HD3  | 48:BZ:116:LEU:HB2 | 1.79                     | 0.64              |
| 1:CA:1301:U:H2'    | 1:CA:1303:C:C5    | 2.32                     | 0.64              |
| 1:CA:194:C:C2'     | 1:CA:195:A:H5''   | 2.27                     | 0.64              |
| 1:CA:740:U:O2'     | 1:CA:741:G:H5'    | 1.97                     | 0.64              |
| 3:CC:100:ALA:O     | 3:CC:101:LEU:HB2  | 1.96                     | 0.64              |
| 4:CD:82:ALA:HB1    | 4:CD:89:THR:CG2   | 2.21                     | 0.64              |
| 1:CA:538:G:H5''    | 12:CL:111:LYS:HD3 | 1.78                     | 0.64              |
| 24:CX:25:C:H2'     | 24:CX:26:G:O4'    | 1.97                     | 0.64              |
| 27:DA:1309:G:C2'   | 27:DA:1310:G:H5'  | 2.27                     | 0.64              |
| 27:DA:1999:C:H4'   | 27:DA:2723:C:O2   | 1.98                     | 0.64              |
| 27:DA:2578:G:N2    | 27:DA:2579:C:C2   | 2.66                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:665:C:H2'    | 27:DA:666:G:C8     | 2.30                     | 0.64              |
| 28:DB:69:G:H2'     | 28:DB:70:C:H6      | 1.62                     | 0.64              |
| 32:DF:63:LYS:O     | 32:DF:64:ILE:C     | 2.35                     | 0.64              |
| 32:DF:74:ARG:O     | 32:DF:75:HIS:CG    | 2.50                     | 0.64              |
| 33:DG:102:PHE:HE2  | 33:DG:141:PHE:HE1  | 1.45                     | 0.64              |
| 36:DN:46:VAL:HG13  | 36:DN:48:MET:HG3   | 1.80                     | 0.64              |
| 40:DR:67:LEU:CD1   | 40:DR:76:VAL:HG21  | 2.27                     | 0.64              |
| 37:DO:77:ILE:HD12  | 42:DT:73:GLU:O     | 1.97                     | 0.64              |
| 1:AA:1257:U:H3'    | 1:AA:1257:U:H6     | 1.63                     | 0.64              |
| 2:AB:71:VAL:O      | 2:AB:165:VAL:HG13  | 1.98                     | 0.64              |
| 3:AC:172:ARG:HE    | 3:AC:203:PHE:HE2   | 1.46                     | 0.64              |
| 8:AH:127:LEU:O     | 8:AH:127:LEU:HD13  | 1.96                     | 0.64              |
| 8:AH:53:VAL:O      | 8:AH:56:LYS:HG3    | 1.98                     | 0.64              |
| 1:AA:1127:G:H5''   | 9:AI:66:ARG:NH2    | 2.13                     | 0.64              |
| 24:AX:6:G:O2'      | 24:AX:7:G:H5'      | 1.98                     | 0.64              |
| 27:BA:1309:G:OP1   | 56:B7:9:ARG:HG3    | 1.97                     | 0.64              |
| 27:BA:176:G:C2'    | 27:BA:177:G:H5'    | 2.28                     | 0.64              |
| 27:BA:572:A:N3     | 27:BA:573:G:H1'    | 2.12                     | 0.64              |
| 27:BA:607:U:OP1    | 32:BF:102:PRO:HA   | 1.98                     | 0.64              |
| 27:BA:99:U:H1'     | 27:BA:102:G:C4     | 2.31                     | 0.64              |
| 28:BB:94:C:H2'     | 28:BB:95:C:H6      | 1.61                     | 0.64              |
| 31:BE:116:VAL:HG21 | 31:BE:122:PHE:CD2  | 2.32                     | 0.64              |
| 35:BI:115:ALA:CB   | 35:BI:129:THR:N    | 2.61                     | 0.64              |
| 39:BQ:85:LYS:HG3   | 49:B0:7:LEU:HB3    | 1.79                     | 0.64              |
| 42:BT:10:VAL:O     | 42:BT:10:VAL:CG1   | 2.46                     | 0.64              |
| 42:BT:89:VAL:CG2   | 42:BT:91:ARG:HH21  | 2.08                     | 0.64              |
| 43:BU:27:LEU:H     | 43:BU:27:LEU:HD23  | 1.61                     | 0.64              |
| 44:BV:19:LYS:HB3   | 44:BV:94:LEU:O     | 1.97                     | 0.64              |
| 45:BW:104:THR:O    | 45:BW:105:VAL:HG23 | 1.98                     | 0.64              |
| 48:BZ:174:VAL:HB   | 48:BZ:175:PRO:CD   | 2.28                     | 0.64              |
| 1:CA:177:C:H2'     | 1:CA:178:C:C6      | 2.33                     | 0.64              |
| 1:CA:577:G:C2      | 1:CA:578:C:C5      | 2.86                     | 0.64              |
| 3:CC:147:LYS:O     | 3:CC:203:PHE:HD2   | 1.81                     | 0.64              |
| 4:CD:103:ASN:O     | 4:CD:106:TYR:HB3   | 1.96                     | 0.64              |
| 5:CE:68:GLU:O      | 5:CE:70:PRO:HD3    | 1.97                     | 0.64              |
| 6:CF:48:LEU:HD13   | 6:CF:52:ILE:HG12   | 1.80                     | 0.64              |
| 7:CG:62:PHE:HA     | 7:CG:124:LEU:HD22  | 1.77                     | 0.64              |
| 17:CQ:95:TYR:HA    | 17:CQ:98:LEU:HD13  | 1.78                     | 0.64              |
| 49:D0:64:ASP:O     | 49:D0:84:LEU:HD11  | 1.98                     | 0.64              |
| 50:D1:40:ARG:HD3   | 50:D1:40:ARG:C     | 2.18                     | 0.64              |
| 53:D4:42:CYS:HA    | 53:D4:59:VAL:HB    | 1.79                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1620:G:C4'   | 56:D7:1:MET:HA     | 2.28                     | 0.64              |
| 27:DA:2555:U:H2'   | 27:DA:2556:C:C5'   | 2.25                     | 0.64              |
| 27:DA:48:G:O2'     | 27:DA:49:A:H5''    | 1.98                     | 0.64              |
| 27:DA:948:G:H2'    | 27:DA:949:C:C6     | 2.33                     | 0.64              |
| 31:DE:119:ARG:HG2  | 31:DE:160:TYR:CD2  | 2.33                     | 0.64              |
| 31:DE:26:ILE:HG13  | 31:DE:182:LEU:HD23 | 1.79                     | 0.64              |
| 33:DG:141:PHE:HB3  | 33:DG:142:PRO:HD2  | 1.80                     | 0.64              |
| 38:DP:18:ARG:HB3   | 38:DP:18:ARG:CZ    | 2.28                     | 0.64              |
| 40:DR:84:ALA:HB3   | 40:DR:85:PRO:HD3   | 1.80                     | 0.64              |
| 48:DZ:43:PHE:CE2   | 48:DZ:85:VAL:HG21  | 2.33                     | 0.64              |
| 1:AA:817:C:C2      | 1:AA:819:A:O4'     | 2.51                     | 0.64              |
| 12:AL:3:THR:H      | 12:AL:6:GLN:NE2    | 1.96                     | 0.64              |
| 13:AM:108:ARG:HH11 | 13:AM:108:ARG:HA   | 1.62                     | 0.64              |
| 13:AM:23:TYR:CE1   | 13:AM:71:ARG:HB2   | 2.33                     | 0.64              |
| 17:AQ:45:HIS:HA    | 17:AQ:69:LYS:HZ1   | 1.61                     | 0.64              |
| 52:B3:23:LEU:O     | 52:B3:28:LEU:N     | 2.29                     | 0.64              |
| 52:B3:59:VAL:CG1   | 52:B3:60:GLU:N     | 2.60                     | 0.64              |
| 55:B6:13:CYS:HA    | 55:B6:50:ARG:O     | 1.96                     | 0.64              |
| 27:BA:1847:A:H4'   | 27:BA:1848:A:OP2   | 1.98                     | 0.64              |
| 27:BA:2165:G:H2'   | 27:BA:2166:G:O4'   | 1.97                     | 0.64              |
| 27:BA:2167:U:H2'   | 27:BA:2168:G:C8    | 2.32                     | 0.64              |
| 27:BA:2225:A:H4'   | 27:BA:2226:C:H6    | 1.62                     | 0.64              |
| 27:BA:685:A:H1'    | 27:BA:688:U:O4     | 1.98                     | 0.64              |
| 27:BA:847:U:H2'    | 27:BA:848:G:C5'    | 2.28                     | 0.64              |
| 29:BC:68:LEU:HD11  | 29:BC:180:PHE:N    | 2.13                     | 0.64              |
| 30:BD:80:ALA:HB3   | 30:BD:94:LEU:O     | 1.96                     | 0.64              |
| 42:BT:34:VAL:O     | 42:BT:35:LYS:HB3   | 1.98                     | 0.64              |
| 1:CA:1026:G:N3     | 1:CA:1026:G:H2'    | 2.13                     | 0.64              |
| 1:CA:1480:G:H2'    | 1:CA:1481:U:H6     | 1.63                     | 0.64              |
| 1:CA:279:A:O2'     | 1:CA:280:C:P       | 2.56                     | 0.64              |
| 1:CA:451:A:H1'     | 1:CA:452:A:C8      | 2.32                     | 0.64              |
| 1:CA:939:G:H5''    | 7:CG:102:ARG:NH1   | 2.12                     | 0.64              |
| 4:CD:172:PRO:HD2   | 4:CD:173:TRP:HZ3   | 1.63                     | 0.64              |
| 4:CD:173:TRP:HE1   | 4:CD:189:PRO:HG3   | 1.57                     | 0.64              |
| 8:CH:87:SER:HB3    | 8:CH:133:LEU:O     | 1.98                     | 0.64              |
| 14:CN:35:ARG:HG3   | 14:CN:36:PHE:N     | 2.13                     | 0.64              |
| 18:CR:36:ASN:H     | 18:CR:36:ASN:ND2   | 1.96                     | 0.64              |
| 55:D6:36:LEU:O     | 55:D6:37:ARG:HD2   | 1.97                     | 0.64              |
| 27:DA:136:G:H1     | 27:DA:143(A):C:N4  | 1.96                     | 0.64              |
| 27:DA:1804:C:H4'   | 30:DD:252:TRP:CZ2  | 2.33                     | 0.64              |
| 27:DA:2850:A:OP2   | 27:DA:2866:U:H5    | 1.80                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DG:105:LYS:HE2  | 53:D4:52:SER:CB    | 2.24                     | 0.64              |
| 33:DG:125:PHE:O    | 33:DG:128:ARG:HG2  | 1.97                     | 0.64              |
| 33:DG:130:ASN:OD1  | 33:DG:160:VAL:HG13 | 1.97                     | 0.64              |
| 37:DO:1:MET:H1     | 37:DO:1:MET:HE2    | 1.63                     | 0.64              |
| 37:DO:40:VAL:HG12  | 37:DO:41:ALA:H     | 1.63                     | 0.64              |
| 43:DU:60:LEU:HD13  | 43:DU:60:LEU:O     | 1.97                     | 0.64              |
| 45:DW:12:ILE:O     | 45:DW:100:THR:HA   | 1.97                     | 0.64              |
| 45:DW:96:ILE:HG13  | 45:DW:97:LYS:N     | 2.12                     | 0.64              |
| 1:AA:1060:C:H2'    | 1:AA:1061:G:H8     | 1.63                     | 0.64              |
| 1:AA:182:U:H6      | 1:AA:182:U:H5'     | 1.62                     | 0.64              |
| 1:AA:316:G:N7      | 1:AA:351:G:C6      | 2.66                     | 0.64              |
| 2:AB:187:LEU:HD11  | 2:AB:204:ASN:O     | 1.98                     | 0.64              |
| 10:AJ:5:ARG:O      | 10:AJ:6:ILE:HG23   | 1.98                     | 0.64              |
| 15:AO:55:GLY:HA2   | 15:AO:58:MET:HE3   | 1.80                     | 0.64              |
| 19:AS:63:THR:HG22  | 19:AS:66:MET:HE2   | 1.79                     | 0.64              |
| 20:AT:14:LYS:HB2   | 20:AT:17:ARG:NH2   | 2.13                     | 0.64              |
| 27:BA:1321:A:H2'   | 27:BA:1322:A:C8    | 2.33                     | 0.64              |
| 27:BA:2065:C:O2'   | 27:BA:2066:C:H5'   | 1.98                     | 0.64              |
| 27:BA:2773:C:O2'   | 27:BA:2774:C:H5'   | 1.98                     | 0.64              |
| 27:BA:2832:U:C4'   | 27:BA:2833:G:H5''  | 2.25                     | 0.64              |
| 27:BA:284:U:H2'    | 27:BA:285:C:H6     | 1.63                     | 0.64              |
| 27:BA:596:G:O2'    | 27:BA:597:U:H5'    | 1.98                     | 0.64              |
| 28:BB:87:G:H3'     | 28:BB:88:C:H5''    | 1.79                     | 0.64              |
| 32:BF:176:LEU:HD11 | 32:BF:180:GLY:CA   | 2.26                     | 0.64              |
| 33:BG:54:GLU:C     | 33:BG:56:ALA:H     | 2.01                     | 0.64              |
| 34:BH:8:PRO:O      | 34:BH:9:ILE:HB     | 1.97                     | 0.64              |
| 27:BA:1162:G:H4'   | 44:BV:24:LYS:HB2   | 1.78                     | 0.64              |
| 44:BV:82:ARG:O     | 44:BV:83:ARG:HG2   | 1.98                     | 0.64              |
| 1:CA:1329:A:OP1    | 13:CM:28:ALA:HB3   | 1.98                     | 0.64              |
| 6:CF:97:PHE:CD2    | 18:CR:31:LEU:HD21  | 2.33                     | 0.64              |
| 14:CN:13:THR:O     | 14:CN:15:LYS:N     | 2.31                     | 0.64              |
| 1:CA:742:G:H5''    | 15:CO:58:MET:HE1   | 1.79                     | 0.64              |
| 50:D1:50:ARG:HG2   | 50:D1:50:ARG:NH1   | 2.12                     | 0.64              |
| 27:DA:1665:A:O2'   | 27:DA:1666:G:H5'   | 1.96                     | 0.64              |
| 27:DA:1838:C:O2'   | 27:DA:1839:G:OP2   | 2.15                     | 0.64              |
| 27:DA:2454:G:O2'   | 27:DA:2455:G:H5'   | 1.98                     | 0.64              |
| 27:DA:436:C:H2'    | 27:DA:437:G:C8     | 2.33                     | 0.64              |
| 27:DA:860:U:H2'    | 27:DA:861:A:H8     | 1.62                     | 0.64              |
| 27:DA:921:G:H4'    | 27:DA:2269:A:C5    | 2.31                     | 0.64              |
| 42:DT:118:ARG:O    | 42:DT:122:ASP:N    | 2.29                     | 0.64              |
| 27:DA:2009:G:OP1   | 45:DW:41:LYS:HE2   | 1.98                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1229:A:O2'   | 1:AA:1230:C:H5'   | 1.98                     | 0.64              |
| 1:AA:1320:C:H42   | 19:AS:36:ARG:HG3  | 1.63                     | 0.64              |
| 1:AA:965:A:H4'    | 1:AA:966:G:OP1    | 1.96                     | 0.64              |
| 7:AG:70:LYS:HB3   | 7:AG:96:GLN:HG2   | 1.80                     | 0.64              |
| 1:AA:1372:U:OP1   | 9:AI:71:SER:HB3   | 1.98                     | 0.64              |
| 10:AJ:16:LEU:HD11 | 10:AJ:70:ARG:HB2  | 1.78                     | 0.64              |
| 57:B8:43:GLN:O    | 57:B8:44:LYS:HD2  | 1.98                     | 0.64              |
| 27:BA:1842:G:H2'  | 27:BA:1843:C:C6   | 2.33                     | 0.64              |
| 27:BA:1973:G:H2'  | 27:BA:1974:C:H6   | 1.63                     | 0.64              |
| 27:BA:309:G:H4'   | 47:BY:18:GLY:HA3  | 1.78                     | 0.64              |
| 28:BB:24:G:H4'    | 28:BB:25:A:O5'    | 1.98                     | 0.64              |
| 30:BD:79:VAL:O    | 30:BD:79:VAL:HG12 | 1.97                     | 0.64              |
| 37:BO:61:VAL:HG12 | 37:BO:87:ILE:HD11 | 1.80                     | 0.64              |
| 42:BT:46:GLU:O    | 42:BT:65:LYS:HB2  | 1.97                     | 0.64              |
| 42:BT:88:ILE:HG22 | 42:BT:89:VAL:N    | 2.09                     | 0.64              |
| 48:BZ:70:VAL:HG22 | 48:BZ:87:PHE:CE2  | 2.33                     | 0.64              |
| 1:CA:810:C:C2'    | 1:CA:811:C:H5'    | 2.28                     | 0.64              |
| 1:CA:901:A:C5     | 1:CA:902:G:H1'    | 2.33                     | 0.64              |
| 1:CA:980:C:H5'    | 1:CA:981:U:H5     | 1.61                     | 0.64              |
| 2:CB:185:ILE:HG23 | 2:CB:199:TYR:CB   | 2.26                     | 0.64              |
| 5:CE:150:ARG:HA   | 5:CE:153:LYS:HE2  | 1.80                     | 0.64              |
| 5:CE:45:PHE:HD1   | 5:CE:46:GLY:N     | 1.96                     | 0.64              |
| 6:CF:43:LEU:H     | 6:CF:43:LEU:HD12  | 1.62                     | 0.64              |
| 9:CI:58:HIS:HB2   | 9:CI:59:PHE:CE1   | 2.33                     | 0.64              |
| 12:CL:109:ASP:O   | 12:CL:111:LYS:HG3 | 1.98                     | 0.64              |
| 15:CO:17:ARG:CZ   | 15:CO:77:ARG:HH12 | 2.10                     | 0.64              |
| 25:CY:63:C:H2'    | 25:CY:64:G:C8     | 2.32                     | 0.64              |
| 27:DA:1137:G:H22  | 36:DN:106:MET:HG2 | 1.63                     | 0.64              |
| 27:DA:1791:A:O2'  | 30:DD:207:GLY:HA2 | 1.97                     | 0.64              |
| 27:DA:637:A:H4'   | 27:DA:638:G:O5'   | 1.97                     | 0.64              |
| 29:DC:18:LYS:HD3  | 29:DC:19:VAL:H    | 1.63                     | 0.64              |
| 30:DD:30:GLU:OE1  | 30:DD:63:ARG:NE   | 2.27                     | 0.64              |
| 32:DF:25:PRO:HB3  | 32:DF:119:ARG:HD3 | 1.79                     | 0.64              |
| 32:DF:66:PRO:O    | 32:DF:68:LYS:N    | 2.31                     | 0.64              |
| 37:DO:6:THR:HG22  | 37:DO:7:TYR:N     | 2.13                     | 0.64              |
| 27:DA:245:G:O5'   | 38:DP:73:GLY:HA2  | 1.98                     | 0.64              |
| 42:DT:16:ARG:NH1  | 42:DT:19:LEU:HD21 | 2.13                     | 0.64              |
| 47:DY:75:ILE:CD1  | 47:DY:79:CYS:HA   | 2.28                     | 0.64              |
| 1:AA:499:A:H4'    | 1:AA:500:G:OP1    | 1.98                     | 0.63              |
| 21:AU:9:ARG:HH11  | 21:AU:22:ARG:HG3  | 1.63                     | 0.63              |
| 55:B6:29:ASN:ND2  | 55:B6:30:THR:HG23 | 2.12                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2261:C:OP2   | 49:B0:17:GLN:OE1   | 2.16                     | 0.63              |
| 27:BA:2488:A:H2'   | 27:BA:2489:G:C8    | 2.33                     | 0.63              |
| 27:BA:554:U:C2'    | 27:BA:555:U:H5'    | 2.28                     | 0.63              |
| 27:BA:582:G:H2'    | 27:BA:583:G:C8     | 2.33                     | 0.63              |
| 27:BA:710:G:O2'    | 27:BA:711:G:H5'    | 1.98                     | 0.63              |
| 30:BD:182:LEU:O    | 30:BD:271:ILE:CG1  | 2.46                     | 0.63              |
| 31:BE:49:LEU:HD13  | 31:BE:81:ILE:HG12  | 1.78                     | 0.63              |
| 27:BA:2635:C:OP1   | 31:BE:77:ILE:HG21  | 1.97                     | 0.63              |
| 35:BI:38:LEU:CD1   | 35:BI:38:LEU:H     | 2.08                     | 0.63              |
| 37:BO:108:GLU:O    | 37:BO:110:GLY:N    | 2.31                     | 0.63              |
| 38:BP:40:SER:O     | 38:BP:41:ARG:HD2   | 1.98                     | 0.63              |
| 41:BS:85:VAL:HG23  | 41:BS:106:ARG:HB2  | 1.78                     | 0.63              |
| 42:BT:19:LEU:HD12  | 42:BT:19:LEU:N     | 2.13                     | 0.63              |
| 47:BY:16:ALA:HA    | 47:BY:21:LYS:HD3   | 1.79                     | 0.63              |
| 47:BY:28:LYS:HA    | 47:BY:39:VAL:H     | 1.63                     | 0.63              |
| 1:CA:1225:A:H2'    | 1:CA:1225:A:N3     | 2.13                     | 0.63              |
| 1:CA:1251:A:H5''   | 9:CI:12:GLU:CD     | 2.18                     | 0.63              |
| 1:CA:1288:A:N1     | 1:CA:1371:G:HI1'   | 2.13                     | 0.63              |
| 1:CA:266:G:H5'     | 1:CA:268:C:H41     | 1.63                     | 0.63              |
| 3:CC:192:THR:O     | 3:CC:192:THR:HG22  | 1.98                     | 0.63              |
| 3:CC:92:ALA:HB2    | 3:CC:99:VAL:HG22   | 1.79                     | 0.63              |
| 8:CH:29:SER:HB3    | 8:CH:32:LYS:HG3    | 1.80                     | 0.63              |
| 8:CH:87:SER:HB2    | 8:CH:93:VAL:HB     | 1.79                     | 0.63              |
| 27:DA:520:G:H2'    | 27:DA:521:G:H8     | 1.60                     | 0.63              |
| 27:DA:557:U:H2'    | 27:DA:558:G:C8     | 2.33                     | 0.63              |
| 30:DD:61:LEU:CB    | 30:DD:63:ARG:HH12  | 2.10                     | 0.63              |
| 31:DE:203:LYS:HE3  | 31:DE:203:LYS:O    | 1.98                     | 0.63              |
| 33:DG:133:LEU:HD12 | 33:DG:134:GLY:N    | 2.13                     | 0.63              |
| 33:DG:135:LEU:HD22 | 33:DG:141:PHE:CE2  | 2.33                     | 0.63              |
| 35:DI:5:LEU:HD12   | 35:DI:17:GLN:O     | 1.97                     | 0.63              |
| 39:DQ:38:GLU:HG3   | 39:DQ:127:ILE:HG22 | 1.79                     | 0.63              |
| 39:DQ:45:GLN:O     | 39:DQ:49:ALA:HB2   | 1.99                     | 0.63              |
| 42:DT:117:ASP:O    | 42:DT:120:ARG:HB2  | 1.97                     | 0.63              |
| 45:DW:68:ARG:CA    | 45:DW:110:LYS:HD3  | 2.28                     | 0.63              |
| 46:DX:36:LYS:HE3   | 46:DX:56:THR:HG23  | 1.80                     | 0.63              |
| 46:DX:57:LEU:HD11  | 46:DX:78:LYS:CG    | 2.28                     | 0.63              |
| 1:AA:1037:C:H2'    | 1:AA:1038:C:C6     | 2.34                     | 0.63              |
| 1:AA:236:G:H5''    | 17:AQ:42:TYR:OH    | 1.97                     | 0.63              |
| 1:AA:471:G:H2'     | 1:AA:472:A:H8      | 1.62                     | 0.63              |
| 2:AB:112:VAL:CG2   | 2:AB:149:LEU:HD13  | 2.23                     | 0.63              |
| 8:AH:97:VAL:HG13   | 8:AH:98:LYS:N      | 2.09                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:48:GLU:N     | 9:AI:49:PRO:HD2    | 2.13                     | 0.63              |
| 10:AJ:8:LEU:HD11  | 10:AJ:23:ILE:HD12  | 1.80                     | 0.63              |
| 12:AL:38:ARG:HH22 | 12:AL:54:LYS:NZ    | 1.95                     | 0.63              |
| 14:AN:26:ARG:HG3  | 14:AN:27:CYS:N     | 2.13                     | 0.63              |
| 15:AO:70:LEU:HD11 | 15:AO:77:ARG:HG3   | 1.80                     | 0.63              |
| 17:AQ:59:ILE:N    | 17:AQ:59:ILE:HD13  | 2.14                     | 0.63              |
| 24:AX:72:A:H3'    | 24:AX:73:A:C8      | 2.29                     | 0.63              |
| 25:AY:57:A:H4'    | 25:AY:58:A:OP1     | 1.95                     | 0.63              |
| 50:B1:46:LEU:N    | 50:B1:46:LEU:HD22  | 2.13                     | 0.63              |
| 50:B1:8:SER:HB3   | 50:B1:66:HIS:CG    | 2.33                     | 0.63              |
| 27:BA:1331:A:H2'  | 27:BA:1333:C:C5    | 2.33                     | 0.63              |
| 27:BA:1603:A:C8   | 27:BA:1603:A:C5'   | 2.79                     | 0.63              |
| 27:BA:1607:C:N4   | 27:BA:1622:G:OP2   | 2.28                     | 0.63              |
| 27:BA:1899:G:N2   | 27:BA:1902:C:N4    | 2.30                     | 0.63              |
| 27:BA:2571:C:H5'' | 27:BA:2572:A:H5''  | 1.80                     | 0.63              |
| 27:BA:2639:A:H2'  | 27:BA:2640:G:O4'   | 1.98                     | 0.63              |
| 27:BA:2700:C:O2'  | 27:BA:2701:C:H5'   | 1.97                     | 0.63              |
| 27:BA:307:G:N2    | 27:BA:310:A:OP2    | 2.32                     | 0.63              |
| 30:BD:31:LYS:CD   | 30:BD:33:LEU:HD13  | 2.28                     | 0.63              |
| 38:BP:97:PRO:C    | 38:BP:98:GLU:HG3   | 2.19                     | 0.63              |
| 39:BQ:12:GLN:CG   | 39:BQ:73:PRO:HD2   | 2.28                     | 0.63              |
| 40:BR:18:LEU:HD11 | 40:BR:22:ARG:NE    | 2.14                     | 0.63              |
| 42:BT:134:GLU:O   | 42:BT:135:ALA:HB3  | 1.98                     | 0.63              |
| 48:BZ:113:GLY:HA3 | 48:BZ:176:PRO:HD3  | 1.80                     | 0.63              |
| 1:CA:1431:C:H2'   | 1:CA:1432:G:O4'    | 1.99                     | 0.63              |
| 1:CA:473:G:H5''   | 16:CP:81:ARG:HH21  | 1.63                     | 0.63              |
| 1:CA:613:C:H2'    | 1:CA:614:A:H8      | 1.63                     | 0.63              |
| 1:CA:831:U:H2'    | 1:CA:832:C:H5'     | 1.79                     | 0.63              |
| 1:CA:878:G:H5'    | 8:CH:89:PRO:HG2    | 1.80                     | 0.63              |
| 1:CA:898:G:N2     | 1:CA:900:A:H3'     | 2.13                     | 0.63              |
| 4:CD:102:ASP:OD1  | 4:CD:103:ASN:N     | 2.31                     | 0.63              |
| 4:CD:156:GLU:O    | 4:CD:160:GLN:HG3   | 1.99                     | 0.63              |
| 1:CA:737:A:O2'    | 6:CF:72:VAL:HG13   | 1.98                     | 0.63              |
| 17:CQ:8:GLY:HA3   | 17:CQ:22:LEU:O     | 1.98                     | 0.63              |
| 52:D3:54:VAL:HG12 | 52:D3:55:ARG:N     | 2.14                     | 0.63              |
| 27:DA:2155:G:H2'  | 27:DA:2156:G:O4'   | 1.96                     | 0.63              |
| 27:DA:2562:U:H1'  | 37:DO:23:ARG:HH12  | 1.63                     | 0.63              |
| 27:DA:271(T):C:H6 | 27:DA:271(T):C:H5' | 1.62                     | 0.63              |
| 30:DD:25:THR:C    | 30:DD:26:LYS:HD3   | 2.19                     | 0.63              |
| 30:DD:32:SER:HA   | 30:DD:36:PRO:HD2   | 1.80                     | 0.63              |
| 30:DD:69:ARG:HD2  | 30:DD:130:ALA:HB2  | 1.79                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DD:71:ASP:CG    | 30:DD:103:ARG:HH22 | 2.01                     | 0.63              |
| 31:DE:144:ARG:HH11 | 31:DE:144:ARG:CG   | 1.99                     | 0.63              |
| 32:DF:99:TYR:HD2   | 32:DF:99:TYR:O     | 1.82                     | 0.63              |
| 34:DH:61:HIS:HA    | 34:DH:64:LEU:HD12  | 1.80                     | 0.63              |
| 36:DN:3:THR:O      | 36:DN:5:VAL:HG12   | 1.98                     | 0.63              |
| 39:DQ:4:PRO:O      | 39:DQ:6:ARG:N      | 2.31                     | 0.63              |
| 42:DT:115:ARG:HA   | 42:DT:115:ARG:HE   | 1.63                     | 0.63              |
| 42:DT:80:SER:O     | 42:DT:81:PRO:C     | 2.36                     | 0.63              |
| 1:AA:1047:G:HO2'   | 1:AA:1215:G:HO2'   | 1.47                     | 0.63              |
| 1:AA:1344:C:O2'    | 1:AA:1345:U:H5'    | 1.97                     | 0.63              |
| 1:AA:178:C:H2'     | 1:AA:179:A:C8      | 2.30                     | 0.63              |
| 1:AA:611:A:H61     | 1:AA:629:G:H1      | 1.44                     | 0.63              |
| 2:AB:224:GLN:HE21  | 2:AB:229:VAL:HG21  | 1.62                     | 0.63              |
| 1:AA:972:C:H4'     | 10:AJ:57:LYS:HG3   | 1.80                     | 0.63              |
| 12:AL:34:CYS:HA    | 12:AL:55:VAL:HG22  | 1.80                     | 0.63              |
| 13:AM:76:ALA:CA    | 13:AM:79:LYS:HZ2   | 2.10                     | 0.63              |
| 14:AN:29:ARG:NH1   | 14:AN:31:ARG:HB2   | 2.12                     | 0.63              |
| 17:AQ:5:VAL:HA     | 17:AQ:59:ILE:O     | 1.97                     | 0.63              |
| 17:AQ:68:ARG:H     | 17:AQ:70:ARG:NH1   | 1.96                     | 0.63              |
| 57:B8:23:VAL:CG1   | 57:B8:46:ARG:HB3   | 2.27                     | 0.63              |
| 27:BA:1820:U:H4'   | 27:BA:1821:A:OP2   | 1.98                     | 0.63              |
| 27:BA:527:C:C4     | 27:BA:2779:U:H2'   | 2.33                     | 0.63              |
| 32:BF:113:ALA:HB1  | 32:BF:186:ILE:HG21 | 1.81                     | 0.63              |
| 34:BH:154:PRO:HG3  | 34:BH:162:ILE:O    | 1.99                     | 0.63              |
| 37:BO:2:ILE:HG21   | 37:BO:8:LEU:HD21   | 1.80                     | 0.63              |
| 27:BA:2880:C:O2'   | 40:BR:90:ARG:NH1   | 2.32                     | 0.63              |
| 41:BS:59:LYS:HZ1   | 41:BS:68:GLN:HE22  | 1.46                     | 0.63              |
| 41:BS:82:ILE:CD1   | 41:BS:82:ILE:H     | 1.97                     | 0.63              |
| 42:BT:13:ARG:O     | 42:BT:15:VAL:N     | 2.27                     | 0.63              |
| 1:CA:110:C:H2'     | 1:CA:111:G:O4'     | 1.99                     | 0.63              |
| 1:CA:1053:G:O6     | 1:CA:1199:U:H2'    | 1.99                     | 0.63              |
| 1:CA:946:A:C6      | 1:CA:1236:A:N1     | 2.67                     | 0.63              |
| 2:CB:19:HIS:HD1    | 2:CB:20:GLU:HG2    | 1.63                     | 0.63              |
| 4:CD:201:GLN:OE1   | 4:CD:204:ILE:HG13  | 1.97                     | 0.63              |
| 9:CI:3:GLN:HG2     | 9:CI:20:ARG:HH12   | 1.64                     | 0.63              |
| 14:CN:7:ILE:O      | 14:CN:10:ALA:HB3   | 1.98                     | 0.63              |
| 15:CO:61:GLY:O     | 15:CO:65:ARG:HD3   | 1.98                     | 0.63              |
| 17:CQ:31:LEU:HD23  | 17:CQ:32:TYR:CZ    | 2.33                     | 0.63              |
| 17:CQ:17:LYS:HG2   | 17:CQ:47:PRO:HA    | 1.80                     | 0.63              |
| 17:CQ:67:LYS:O     | 17:CQ:68:ARG:HB3   | 1.98                     | 0.63              |
| 19:CS:19:VAL:O     | 19:CS:23:ASN:HB3   | 1.97                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:CS:63:THR:HG22  | 19:CS:66:MET:HG2   | 1.80                     | 0.63              |
| 25:CY:65:U:H2'     | 25:CY:66:A:H8      | 1.63                     | 0.63              |
| 50:D1:67:ILE:N     | 50:D1:68:PRO:CD    | 2.62                     | 0.63              |
| 50:D1:7:ILE:HD13   | 50:D1:62:VAL:HB    | 1.79                     | 0.63              |
| 27:DA:1388:G:C2'   | 27:DA:1389:G:H5'   | 2.27                     | 0.63              |
| 27:DA:1899:G:N2    | 27:DA:1902:C:N4    | 2.46                     | 0.63              |
| 27:DA:2476:A:H2'   | 27:DA:2477:C:H5''  | 1.79                     | 0.63              |
| 27:DA:428:A:H3'    | 27:DA:429:A:C8     | 2.34                     | 0.63              |
| 27:DA:571:A:H1'    | 27:DA:573:G:C8     | 2.34                     | 0.63              |
| 27:DA:614(C):A:H4' | 27:DA:615:G:OP1    | 1.97                     | 0.63              |
| 27:DA:95:G:HO2'    | 51:D2:48:HIS:HD1   | 1.46                     | 0.63              |
| 27:DA:97:C:H4'     | 51:D2:2:LYS:CB     | 2.25                     | 0.63              |
| 30:DD:67:PHE:CZ    | 30:DD:157:ARG:NE   | 2.64                     | 0.63              |
| 31:DE:15:PHE:CZ    | 42:DT:80:SER:HB2   | 2.34                     | 0.63              |
| 32:DF:53:THR:HG23  | 32:DF:55:GLY:H     | 1.62                     | 0.63              |
| 32:DF:9:ILE:HG12   | 32:DF:14:PRO:HA    | 1.81                     | 0.63              |
| 33:DG:32:PRO:HB2   | 33:DG:172:LEU:HD13 | 1.79                     | 0.63              |
| 33:DG:47:LYS:N     | 33:DG:51:ARG:HG3   | 2.14                     | 0.63              |
| 27:DA:2746:U:H1'   | 34:DH:139:GLN:HB3  | 1.80                     | 0.63              |
| 37:DO:101:PRO:HD3  | 42:DT:67:SER:O     | 1.98                     | 0.63              |
| 38:DP:123:LEU:HD12 | 38:DP:125:VAL:CG1  | 2.27                     | 0.63              |
| 39:DQ:63:LYS:HG2   | 39:DQ:64:ILE:N     | 2.13                     | 0.63              |
| 43:DU:14:HIS:C     | 43:DU:16:LYS:H     | 2.02                     | 0.63              |
| 1:AA:1171:G:H2'    | 1:AA:1172:C:C6     | 2.33                     | 0.63              |
| 1:AA:189(E):U:O2   | 1:AA:189(E):U:H2'  | 1.98                     | 0.63              |
| 1:AA:595:G:H1      | 1:AA:641:U:H2'     | 1.64                     | 0.63              |
| 3:AC:16:ARG:CB     | 3:AC:16:ARG:HH11   | 2.07                     | 0.63              |
| 12:AL:89:ASP:O     | 12:AL:91:PRO:HD3   | 1.98                     | 0.63              |
| 51:B2:42:GLY:O     | 51:B2:44:LEU:N     | 2.31                     | 0.63              |
| 27:BA:1241:A:O2'   | 27:BA:1242:A:H5'   | 1.98                     | 0.63              |
| 27:BA:1412:A:H2'   | 27:BA:1413:G:H8    | 1.60                     | 0.63              |
| 27:BA:1439:A:C2    | 27:BA:1553:A:C4    | 2.87                     | 0.63              |
| 27:BA:1658:C:H2'   | 27:BA:1659:U:H6    | 1.64                     | 0.63              |
| 27:BA:197:A:C8     | 27:BA:197:A:H5'    | 2.26                     | 0.63              |
| 27:BA:2228:G:P     | 30:BD:263:ARG:HH12 | 2.21                     | 0.63              |
| 27:BA:2270:G:H2'   | 27:BA:2271:G:O4'   | 1.97                     | 0.63              |
| 27:BA:2321:G:O2'   | 27:BA:2322:A:H5'   | 1.98                     | 0.63              |
| 27:BA:2684:U:O2'   | 37:BO:68:GLU:HG3   | 1.98                     | 0.63              |
| 27:BA:49:A:H5''    | 27:BA:51:G:O4'     | 1.99                     | 0.63              |
| 32:BF:40:GLN:NE2   | 32:BF:184:TYR:HB3  | 2.14                     | 0.63              |
| 33:BG:128:ARG:C    | 33:BG:130:ASN:N    | 2.48                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BQ:79:LEU:HD12  | 39:BQ:79:LEU:N    | 2.12                     | 0.63              |
| 40:BR:22:ARG:O     | 40:BR:25:ALA:N    | 2.32                     | 0.63              |
| 42:BT:122:ASP:O    | 42:BT:124:ASP:N   | 2.31                     | 0.63              |
| 42:BT:33:LYS:HE3   | 42:BT:74:ARG:NH2  | 2.14                     | 0.63              |
| 47:BY:26:LYS:HG2   | 47:BY:27:VAL:HG23 | 1.80                     | 0.63              |
| 1:CA:1032:G:H2'    | 1:CA:1033:G:C8    | 2.34                     | 0.63              |
| 1:CA:1038:C:H2'    | 1:CA:1039:C:C4    | 2.32                     | 0.63              |
| 1:CA:297:G:N2      | 1:CA:300:A:OP2    | 2.32                     | 0.63              |
| 2:CB:91:PRO:CG     | 2:CB:154:LEU:HB2  | 2.16                     | 0.63              |
| 8:CH:10:LEU:CD2    | 8:CH:83:ILE:HG12  | 2.26                     | 0.63              |
| 24:CX:37:A:H3'     | 24:CX:38:A:H8     | 1.63                     | 0.63              |
| 25:CY:38:U:O2      | 25:CY:38:U:H3'    | 1.97                     | 0.63              |
| 27:DA:2262:U:P     | 49:D0:19:LYS:HZ2  | 2.22                     | 0.63              |
| 50:D1:80:LEU:HB3   | 50:D1:82:LEU:HD21 | 1.78                     | 0.63              |
| 27:DA:2039:C:OP2   | 36:DN:109:LYS:HD3 | 1.97                     | 0.63              |
| 27:DA:2078:C:O2'   | 27:DA:2079:U:H5'  | 1.99                     | 0.63              |
| 27:DA:2064:C:H1'   | 27:DA:2450:A:C6   | 2.34                     | 0.63              |
| 27:DA:55:G:H2'     | 27:DA:56:A:C8     | 2.31                     | 0.63              |
| 28:DB:87:G:H3'     | 28:DB:88:C:C5'    | 2.28                     | 0.63              |
| 30:DD:35:LYS:CB    | 30:DD:36:PRO:HD3  | 2.29                     | 0.63              |
| 36:DN:82:LEU:HD12  | 36:DN:83:LYS:N    | 2.14                     | 0.63              |
| 40:DR:83:ILE:O     | 40:DR:86:ARG:HG3  | 1.98                     | 0.63              |
| 3:AC:43:LEU:HB3    | 3:AC:47:LEU:HD23  | 1.81                     | 0.63              |
| 5:AE:81:GLU:HG2    | 5:AE:90:VAL:HG12  | 1.80                     | 0.63              |
| 6:AF:69:GLU:O      | 6:AF:72:VAL:HG12  | 1.98                     | 0.63              |
| 11:AK:122:LYS:O    | 11:AK:126:ARG:HG3 | 1.99                     | 0.63              |
| 1:AA:528:C:H41     | 12:AL:46:ASN:CG   | 2.02                     | 0.63              |
| 1:AA:1228:C:H4'    | 13:AM:116:THR:CA  | 2.29                     | 0.63              |
| 13:AM:14:ARG:HD2   | 13:AM:42:ALA:O    | 1.97                     | 0.63              |
| 14:AN:15:LYS:O     | 14:AN:16:PHE:O    | 2.16                     | 0.63              |
| 20:AT:29:LYS:O     | 20:AT:32:ALA:HB3  | 1.98                     | 0.63              |
| 27:BA:125:G:H21    | 56:B7:48:LYS:HZ2  | 1.45                     | 0.63              |
| 27:BA:1375:C:H2'   | 27:BA:1376:C:H6   | 1.64                     | 0.63              |
| 27:BA:1654:A:OP2   | 40:BR:3:HIS:HB2   | 1.98                     | 0.63              |
| 27:BA:1945:G:H2'   | 27:BA:1946:U:C6   | 2.33                     | 0.63              |
| 27:BA:492:A:H2'    | 27:BA:493:G:O4'   | 1.98                     | 0.63              |
| 27:BA:508:G:N3     | 27:BA:508:G:H2'   | 2.12                     | 0.63              |
| 27:BA:723:G:O2'    | 27:BA:724:U:H5'   | 1.98                     | 0.63              |
| 32:BF:160:ASN:HD22 | 32:BF:160:ASN:C   | 2.02                     | 0.63              |
| 32:BF:70:THR:C     | 32:BF:72:ARG:H    | 2.01                     | 0.63              |
| 34:BH:86:GLU:HG2   | 34:BH:86:GLU:O    | 1.98                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BH:8:PRO:HD2    | 34:BH:69:ARG:CD    | 2.24                     | 0.63              |
| 37:BO:114:ILE:N    | 37:BO:114:ILE:HD13 | 2.13                     | 0.63              |
| 27:BA:1155:A:OP1   | 43:BU:55:ARG:HD2   | 1.98                     | 0.63              |
| 47:BY:31:LEU:HD22  | 47:BY:31:LEU:N     | 2.14                     | 0.63              |
| 1:CA:1442(A):G:H5' | 1:CA:1442(B):A:OP2 | 1.99                     | 0.63              |
| 3:CC:156:ARG:NH2   | 3:CC:161:GLU:HG3   | 2.12                     | 0.63              |
| 4:CD:121:VAL:HG22  | 4:CD:126:ILE:HG13  | 1.79                     | 0.63              |
| 8:CH:123:GLU:O     | 8:CH:127:LEU:HB2   | 1.97                     | 0.63              |
| 7:CG:150:ALA:HB2   | 11:CK:50:TYR:CZ    | 2.34                     | 0.63              |
| 20:CT:86:ARG:HH11  | 20:CT:86:ARG:HG3   | 1.63                     | 0.63              |
| 56:D7:24:THR:HG23  | 56:D7:27:GLY:N     | 2.13                     | 0.63              |
| 57:D8:16:ILE:CG2   | 57:D8:64:TYR:HB3   | 2.28                     | 0.63              |
| 27:DA:1032:A:O3'   | 58:D9:16:VAL:HG11  | 1.99                     | 0.63              |
| 27:DA:1012:U:O4    | 36:DN:25:ARG:HA    | 1.99                     | 0.63              |
| 27:DA:1273:U:C6    | 27:DA:1273:U:H5''  | 2.27                     | 0.63              |
| 27:DA:1497:U:H5'   | 27:DA:1498:C:C5    | 2.31                     | 0.63              |
| 27:DA:1718:G:H1    | 27:DA:1744:C:N4    | 1.92                     | 0.63              |
| 27:DA:2429:G:OP2   | 27:DA:2430:A:OP2   | 2.17                     | 0.63              |
| 27:DA:2503:A:H4'   | 27:DA:2504:U:OP1   | 1.99                     | 0.63              |
| 27:DA:2833:G:C3'   | 27:DA:2834:G:H5''  | 2.07                     | 0.63              |
| 30:DD:43:ARG:HD2   | 30:DD:44:ASN:CG    | 2.18                     | 0.63              |
| 32:DF:21:ALA:O     | 32:DF:24:LEU:HB2   | 1.99                     | 0.63              |
| 36:DN:43:THR:HB    | 36:DN:46:VAL:HG12  | 1.80                     | 0.63              |
| 40:DR:4:LEU:O      | 40:DR:4:LEU:HD13   | 1.99                     | 0.63              |
| 42:DT:62:THR:HG22  | 42:DT:75:ILE:CG1   | 2.28                     | 0.63              |
| 43:DU:83:LEU:HG    | 43:DU:88:ILE:CD1   | 2.27                     | 0.63              |
| 44:DV:19:LYS:HZ3   | 44:DV:20:LEU:H     | 1.45                     | 0.63              |
| 48:DZ:47:PHE:O     | 48:DZ:51:SER:N     | 2.31                     | 0.63              |
| 1:AA:1064:G:O2'    | 1:AA:1190:G:N2     | 2.32                     | 0.63              |
| 6:AF:38:GLU:O      | 6:AF:39:LYS:HB2    | 1.99                     | 0.63              |
| 9:AI:4:TYR:CD1     | 9:AI:4:TYR:N       | 2.60                     | 0.63              |
| 1:AA:1308:U:H5'    | 13:AM:110:ARG:HD2  | 1.80                     | 0.63              |
| 20:AT:98:PRO:C     | 20:AT:100:ILE:H    | 2.01                     | 0.63              |
| 50:B1:37:ILE:CG2   | 50:B1:38:SER:H     | 1.94                     | 0.63              |
| 57:B8:32:LEU:HB3   | 57:B8:36:LYS:CE    | 2.28                     | 0.63              |
| 27:BA:1175:U:H6    | 27:BA:1178:C:H42   | 1.47                     | 0.63              |
| 27:BA:1777:U:H2'   | 27:BA:1778:U:H6    | 1.63                     | 0.63              |
| 27:BA:1924:C:C2'   | 27:BA:1925:C:H5'   | 2.29                     | 0.63              |
| 27:BA:192:C:H2'    | 27:BA:193:U:H5'    | 1.80                     | 0.63              |
| 27:BA:2096:U:H2'   | 27:BA:2097:C:H6    | 1.62                     | 0.63              |
| 27:BA:218:A:C2     | 27:BA:235:U:H4'    | 2.33                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1750:G:O2'   | 27:BA:2860:A:N1    | 2.32                     | 0.63              |
| 27:BA:304:G:H2'    | 27:BA:305:U:C6     | 2.34                     | 0.63              |
| 30:BD:165:ILE:CD1  | 30:BD:175:LEU:HD21 | 2.16                     | 0.63              |
| 30:BD:241:PRO:O    | 30:BD:242:ARG:CB   | 2.44                     | 0.63              |
| 31:BE:119:ARG:HD2  | 31:BE:120:TRP:CE2  | 2.34                     | 0.63              |
| 40:BR:111:LEU:N    | 40:BR:111:LEU:HD22 | 2.13                     | 0.63              |
| 44:BV:99:ILE:H     | 44:BV:99:ILE:HD13  | 1.63                     | 0.63              |
| 48:BZ:18:ARG:NH1   | 48:BZ:83:GLU:O     | 2.31                     | 0.63              |
| 1:CA:1348:U:H2'    | 1:CA:1349:A:H8     | 1.63                     | 0.63              |
| 1:CA:32:A:C2       | 1:CA:33:A:C4       | 2.87                     | 0.63              |
| 3:CC:156:ARG:HE    | 3:CC:161:GLU:HA    | 1.62                     | 0.63              |
| 10:CJ:5:ARG:HG3    | 10:CJ:71:LEU:HD11  | 1.79                     | 0.63              |
| 6:CF:100:ASN:HB3   | 18:CR:27:GLY:O     | 1.98                     | 0.63              |
| 20:CT:104:LEU:HD23 | 20:CT:105:SER:N    | 2.13                     | 0.63              |
| 27:DA:118:A:H5'    | 27:DA:119:A:C8     | 2.33                     | 0.63              |
| 27:DA:1838:C:N3    | 27:DA:1901:A:N6    | 2.46                     | 0.63              |
| 27:DA:2180:U:H2'   | 27:DA:2181:G:C8    | 2.34                     | 0.63              |
| 27:DA:90:U:H2'     | 27:DA:90:U:O2      | 1.96                     | 0.63              |
| 27:DA:953:A:OP2    | 39:DQ:16:ARG:NH2   | 2.31                     | 0.63              |
| 27:DA:975(A):G:O2' | 27:DA:976:C:H5'    | 1.98                     | 0.63              |
| 28:DB:30:C:H2'     | 28:DB:31:C:O4'     | 1.98                     | 0.63              |
| 31:DE:102:VAL:HG13 | 31:DE:172:VAL:CG2  | 2.29                     | 0.63              |
| 31:DE:33:VAL:HG22  | 31:DE:69:LYS:HE3   | 1.80                     | 0.63              |
| 33:DG:11:TYR:HE1   | 33:DG:172:LEU:HD11 | 1.63                     | 0.63              |
| 33:DG:27:ASN:O     | 33:DG:28:VAL:HB    | 1.99                     | 0.63              |
| 35:DI:9:LEU:O      | 35:DI:13:GLY:CA    | 2.47                     | 0.63              |
| 42:DT:102:ILE:HB   | 42:DT:110:ILE:HD11 | 1.81                     | 0.63              |
| 42:DT:23:ARG:HE    | 42:DT:120:ARG:HH11 | 1.45                     | 0.63              |
| 42:DT:33:LYS:HB2   | 42:DT:41:ARG:HB3   | 1.80                     | 0.63              |
| 43:DU:5:LYS:HG2    | 43:DU:7:GLY:H      | 1.62                     | 0.63              |
| 47:DY:4:LYS:HG3    | 47:DY:5:MET:H      | 1.63                     | 0.63              |
| 1:AA:1030(A):G:H1' | 1:AA:1031:G:H22    | 1.63                     | 0.63              |
| 1:AA:190:U:O2'     | 1:AA:191:G:H5'     | 1.98                     | 0.63              |
| 2:AB:218:ALA:O     | 2:AB:222:ILE:HG13  | 1.99                     | 0.63              |
| 9:AI:28:VAL:HA     | 9:AI:63:ILE:O      | 1.99                     | 0.63              |
| 10:AJ:9:ARG:O      | 10:AJ:94:VAL:HG13  | 1.99                     | 0.63              |
| 11:AK:124:LYS:HB2  | 11:AK:125:PHE:CD1  | 2.34                     | 0.63              |
| 27:BA:1316:U:O2'   | 27:BA:1317:A:H5'   | 1.98                     | 0.63              |
| 27:BA:96:G:H4'     | 51:B2:48:HIS:HD2   | 1.63                     | 0.63              |
| 31:BE:184:VAL:CG1  | 31:BE:185:LYS:H    | 2.12                     | 0.63              |
| 34:BH:152:ARG:HB2  | 34:BH:162:ILE:HG13 | 1.80                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BI:113:ARG:O    | 35:BI:130:TYR:HD1 | 1.82                     | 0.63              |
| 36:BN:56:ASN:HA    | 36:BN:125:GLY:H   | 1.63                     | 0.63              |
| 38:BP:29:LYS:HB3   | 38:BP:34:GLY:H    | 1.63                     | 0.63              |
| 40:BR:79:LEU:HA    | 40:BR:83:ILE:CG1  | 2.22                     | 0.63              |
| 46:BX:12:VAL:CG1   | 46:BX:27:THR:HG23 | 2.29                     | 0.63              |
| 46:BX:12:VAL:HG23  | 46:BX:13:LEU:N    | 2.13                     | 0.63              |
| 1:CA:1027:C:H2'    | 1:CA:1028:C:C5    | 2.33                     | 0.63              |
| 1:CA:1308:U:OP1    | 13:CM:97:PRO:HA   | 1.98                     | 0.63              |
| 1:CA:291:C:O2'     | 1:CA:292:G:H5'    | 1.99                     | 0.63              |
| 2:CB:22:LYS:O      | 2:CB:24:TRP:HD1   | 1.82                     | 0.63              |
| 3:CC:77:ILE:HG22   | 3:CC:81:GLY:HA2   | 1.80                     | 0.63              |
| 5:CE:88:LYS:HD3    | 5:CE:123:LEU:HD12 | 1.79                     | 0.63              |
| 1:CA:1280:A:H5''   | 10:CJ:40:LEU:HD12 | 1.80                     | 0.63              |
| 13:CM:3:ARG:HG2    | 13:CM:9:ILE:HG13  | 1.81                     | 0.63              |
| 27:DA:1819:A:H5''  | 30:DD:158:ALA:HB2 | 1.80                     | 0.63              |
| 27:DA:2165:G:H2'   | 27:DA:2166:G:C8   | 2.33                     | 0.63              |
| 27:DA:811:U:O2     | 27:DA:1250:G:H3'  | 1.98                     | 0.63              |
| 28:DB:17:C:H2'     | 28:DB:18:G:H8     | 1.63                     | 0.63              |
| 29:DC:47:LEU:H     | 29:DC:47:LEU:HD23 | 1.62                     | 0.63              |
| 32:DF:117:ARG:HH21 | 32:DF:187:VAL:HA  | 1.64                     | 0.63              |
| 37:DO:103:ALA:HB1  | 37:DO:105:GLU:OE1 | 1.99                     | 0.63              |
| 27:DA:2275:C:O2'   | 39:DQ:85:LYS:N    | 2.32                     | 0.63              |
| 40:DR:100:LEU:HD21 | 40:DR:113:LEU:HB2 | 1.80                     | 0.63              |
| 36:DN:4:TYR:CB     | 43:DU:64:ARG:HH22 | 2.12                     | 0.63              |
| 27:DA:1151:G:H5''  | 43:DU:81:HIS:CE1  | 2.33                     | 0.63              |
| 43:DU:90:VAL:HG12  | 43:DU:91:ASP:N    | 2.08                     | 0.63              |
| 45:DW:83:LYS:HG2   | 45:DW:97:LYS:CD   | 2.29                     | 0.63              |
| 47:DY:28:LYS:H     | 47:DY:28:LYS:HZ2  | 1.46                     | 0.63              |
| 1:AA:1203:C:H2'    | 1:AA:1204:A:H8    | 1.64                     | 0.63              |
| 1:AA:52:G:O2'      | 1:AA:53:A:H8      | 1.81                     | 0.63              |
| 1:AA:762:C:H2'     | 1:AA:763:G:H8     | 1.63                     | 0.63              |
| 1:AA:853:G:O2'     | 1:AA:854:G:H5'    | 1.99                     | 0.63              |
| 2:AB:233:SER:OG    | 2:AB:234:PRO:HD2  | 1.98                     | 0.63              |
| 3:AC:143:GLU:C     | 3:AC:145:GLY:H    | 2.00                     | 0.63              |
| 12:AL:25:LYS:O     | 12:AL:26:GLY:C    | 2.37                     | 0.63              |
| 13:AM:17:VAL:HA    | 13:AM:20:THR:OG1  | 1.99                     | 0.63              |
| 13:AM:81:LEU:HB3   | 13:AM:89:GLY:HA2  | 1.81                     | 0.63              |
| 14:AN:45:ARG:O     | 14:AN:45:ARG:HG2  | 1.99                     | 0.63              |
| 24:AX:29:G:H2'     | 24:AX:30:G:H8     | 1.64                     | 0.63              |
| 27:BA:2886:G:O2'   | 54:B5:32:PRO:HD2  | 1.99                     | 0.63              |
| 27:BA:1252:G:H4'   | 27:BA:1253:A:OP1  | 1.99                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1290:C:H2'   | 27:BA:1291:C:C6    | 2.33                     | 0.63              |
| 27:BA:1804:C:O2'   | 27:BA:1805:U:H5'   | 1.98                     | 0.63              |
| 27:BA:557:U:O2'    | 27:BA:558:G:H5'    | 1.98                     | 0.63              |
| 30:BD:25:THR:O     | 30:BD:26:LYS:HD3   | 1.98                     | 0.63              |
| 36:BN:133:GLN:C    | 36:BN:134:ARG:HG3  | 2.17                     | 0.63              |
| 38:BP:144:GLU:N    | 38:BP:145:PRO:CD   | 2.62                     | 0.63              |
| 39:BQ:115:MET:CE   | 39:BQ:131:ILE:HG21 | 2.28                     | 0.63              |
| 39:BQ:58:PHE:CD1   | 39:BQ:58:PHE:O     | 2.51                     | 0.63              |
| 41:BS:68:GLN:HG2   | 41:BS:71:ARG:NH1   | 2.14                     | 0.63              |
| 44:BV:15:GLU:CB    | 44:BV:16:PRO:HD2   | 2.28                     | 0.63              |
| 47:BY:81:LYS:HZ3   | 47:BY:97:ARG:HG2   | 1.61                     | 0.63              |
| 48:BZ:157:PRO:O    | 48:BZ:160:VAL:HB   | 1.99                     | 0.63              |
| 48:BZ:68:THR:HA    | 48:BZ:90:LEU:HD12  | 1.80                     | 0.63              |
| 1:CA:186:C:H2'     | 1:CA:187:C:C6      | 2.33                     | 0.63              |
| 1:CA:298:A:H2'     | 1:CA:299:G:O4'     | 1.98                     | 0.63              |
| 1:CA:377:G:H2'     | 1:CA:378:G:C8      | 2.34                     | 0.63              |
| 1:CA:980:C:H3'     | 1:CA:981:U:C6      | 2.34                     | 0.63              |
| 3:CC:89:GLU:OE2    | 3:CC:93:LYS:HD2    | 1.99                     | 0.63              |
| 4:CD:49:ARG:HD3    | 4:CD:50:ARG:N      | 2.14                     | 0.63              |
| 7:CG:50:ILE:HD11   | 7:CG:121:ALA:HA    | 1.80                     | 0.63              |
| 16:CP:74:LEU:O     | 16:CP:79:VAL:HG23  | 1.99                     | 0.63              |
| 19:CS:33:THR:O     | 19:CS:57:HIS:HE1   | 1.81                     | 0.63              |
| 1:CA:1492:A:H5'    | 26:CZ:6:5OH:HP     | 1.80                     | 0.63              |
| 49:D0:72:ARG:HE    | 49:D0:75:LEU:HD12  | 1.63                     | 0.63              |
| 45:DW:23:LEU:HD21  | 54:D5:25:LEU:HD13  | 1.81                     | 0.63              |
| 57:D8:14:VAL:CG2   | 57:D8:22:VAL:HG13  | 2.24                     | 0.63              |
| 27:DA:2382:G:O2'   | 27:DA:2383:G:OP2   | 2.14                     | 0.63              |
| 32:DF:155:LEU:HD11 | 32:DF:176:LEU:HD23 | 1.80                     | 0.63              |
| 33:DG:112:PRO:C    | 33:DG:113:ARG:HH11 | 2.00                     | 0.63              |
| 38:DP:16:ARG:NH2   | 38:DP:18:ARG:HG3   | 2.13                     | 0.63              |
| 39:DQ:66:ILE:O     | 39:DQ:66:ILE:CG1   | 2.46                     | 0.63              |
| 41:DS:82:ILE:HG22  | 41:DS:83:LYS:N     | 2.14                     | 0.63              |
| 1:AA:1073:U:H3     | 1:AA:1102:A:H61    | 1.46                     | 0.63              |
| 1:AA:1404:C:H2'    | 1:AA:1405:G:C8     | 2.34                     | 0.63              |
| 1:AA:503:C:O2'     | 1:AA:504:C:H5'     | 1.99                     | 0.63              |
| 1:AA:545:C:H5''    | 4:AD:72:GLU:HG2    | 1.81                     | 0.63              |
| 4:AD:65:ARG:HD2    | 4:AD:72:GLU:HA     | 1.81                     | 0.63              |
| 12:AL:35:THR:OG1   | 12:AL:36:VAL:HG23  | 1.99                     | 0.63              |
| 20:AT:79:ARG:HH21  | 20:AT:80:ARG:NH2   | 1.97                     | 0.63              |
| 24:AX:53:G:H2'     | 24:AX:54:U:C6      | 2.33                     | 0.63              |
| 55:B6:14:THR:O     | 55:B6:49:HIS:HA    | 1.98                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1686:C:H2'   | 27:BA:1687:G:O4'   | 1.99                     | 0.63              |
| 27:BA:2158:A:O2'   | 27:BA:2159:G:H8    | 1.82                     | 0.63              |
| 27:BA:221:A:H4'    | 27:BA:222:A:O5'    | 1.98                     | 0.63              |
| 27:BA:702:G:O2'    | 27:BA:703:U:H5'    | 1.99                     | 0.63              |
| 32:BF:7:TYR:O      | 32:BF:15:SER:HB2   | 1.99                     | 0.63              |
| 34:BH:88:LEU:CD1   | 34:BH:130:ARG:HG3  | 2.29                     | 0.63              |
| 35:BI:144:VAL:HG23 | 35:BI:145:VAL:HG23 | 1.80                     | 0.63              |
| 39:BQ:51:ARG:NH1   | 39:BQ:52:VAL:HG23  | 2.14                     | 0.63              |
| 41:BS:105:ALA:C    | 41:BS:107:GLU:N    | 2.52                     | 0.63              |
| 42:BT:108:ARG:HA   | 42:BT:111:ARG:HG3  | 1.81                     | 0.63              |
| 44:BV:62:LEU:N     | 44:BV:62:LEU:HD22  | 2.13                     | 0.63              |
| 47:BY:50:ARG:HD2   | 47:BY:56:PRO:O     | 1.99                     | 0.63              |
| 47:BY:8:LYS:HD2    | 47:BY:8:LYS:N      | 2.14                     | 0.63              |
| 1:CA:992:U:H3      | 1:CA:1044:A:H62    | 1.45                     | 0.63              |
| 1:CA:1423:G:H2'    | 1:CA:1424:C:H6     | 1.64                     | 0.63              |
| 1:CA:189(K):U:H2'  | 1:CA:189(L):G:C8   | 2.34                     | 0.63              |
| 1:CA:472:A:C4'     | 16:CP:82:GLN:HE22  | 2.12                     | 0.63              |
| 2:CB:76:GLN:O      | 2:CB:208:ILE:HG12  | 1.99                     | 0.63              |
| 4:CD:26:CYS:HA     | 4:CD:31:CYS:HA     | 1.81                     | 0.63              |
| 13:CM:23:TYR:CD1   | 13:CM:71:ARG:HB2   | 2.34                     | 0.63              |
| 49:D0:5:LYS:HB3    | 49:D0:5:LYS:HZ2    | 1.64                     | 0.63              |
| 27:DA:1909:C:H42   | 27:DA:1921:G:H1    | 1.47                     | 0.63              |
| 27:DA:1917:U:H2'   | 27:DA:1918:A:H8    | 1.62                     | 0.63              |
| 27:DA:272:G:O6     | 27:DA:421:U:H2'    | 1.99                     | 0.63              |
| 27:DA:940:G:H2'    | 27:DA:941:A:H5''   | 1.81                     | 0.63              |
| 27:DA:967:C:O2'    | 27:DA:968:G:H5'    | 1.99                     | 0.63              |
| 28:DB:26:A:H3'     | 28:DB:27:C:H5''    | 1.81                     | 0.63              |
| 30:DD:26:LYS:HZ1   | 30:DD:82:ILE:N     | 1.97                     | 0.63              |
| 31:DE:33:VAL:HG23  | 31:DE:69:LYS:HE3   | 1.81                     | 0.63              |
| 37:DO:68:GLU:HA    | 37:DO:77:ILE:O     | 1.99                     | 0.63              |
| 38:DP:16:ARG:CZ    | 38:DP:18:ARG:HG3   | 2.28                     | 0.63              |
| 38:DP:90:ARG:HB3   | 38:DP:91:PHE:HD1   | 1.63                     | 0.63              |
| 39:DQ:33:GLY:HA2   | 39:DQ:105:GLU:HA   | 1.80                     | 0.63              |
| 47:DY:81:LYS:HD3   | 47:DY:97:ARG:CB    | 2.22                     | 0.63              |
| 1:AA:1136:U:H5''   | 1:AA:1137:C:C6     | 2.34                     | 0.62              |
| 1:AA:1239:A:H62    | 1:AA:1299:A:N6     | 1.95                     | 0.62              |
| 1:AA:1371:G:H2'    | 1:AA:1372:U:C6     | 2.34                     | 0.62              |
| 1:AA:1375:A:H2'    | 1:AA:1376:U:O4'    | 2.00                     | 0.62              |
| 1:AA:781:A:H4'     | 1:AA:1522:U:O2'    | 1.99                     | 0.62              |
| 2:AB:32:ILE:HG12   | 2:AB:33:TYR:N      | 2.13                     | 0.62              |
| 53:B4:40:ILE:C     | 53:B4:41:ILE:HD13  | 2.19                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:BP:49:ARG:HD2   | 57:B8:59:LYS:CG   | 2.28                     | 0.62              |
| 27:BA:1023:U:H2'   | 27:BA:1024:G:C5'  | 2.28                     | 0.62              |
| 27:BA:1154:G:O5'   | 27:BA:1154:G:H8   | 1.82                     | 0.62              |
| 27:BA:1690:A:H2'   | 27:BA:1691:C:O4'  | 1.99                     | 0.62              |
| 27:BA:2181:G:O2'   | 27:BA:2182:G:H5'  | 1.99                     | 0.62              |
| 27:BA:2628:C:O2'   | 27:BA:2781:A:H2'  | 1.98                     | 0.62              |
| 27:BA:2732:G:H3'   | 27:BA:2733:A:H5'  | 1.81                     | 0.62              |
| 27:BA:2863:C:C3'   | 27:BA:2864:G:H5'' | 2.29                     | 0.62              |
| 27:BA:286:C:O2'    | 27:BA:287:C:H5'   | 1.99                     | 0.62              |
| 27:BA:71:A:H5''    | 27:BA:73:A:N7     | 2.14                     | 0.62              |
| 27:BA:919:G:O2'    | 27:BA:920:G:H5'   | 1.99                     | 0.62              |
| 27:BA:955:C:OP1    | 39:BQ:87:LYS:HE2  | 1.98                     | 0.62              |
| 29:BC:83:ILE:HD11  | 29:BC:95:GLY:O    | 1.98                     | 0.62              |
| 27:BA:1815:A:OP2   | 30:BD:54:ARG:NH1  | 2.31                     | 0.62              |
| 31:BE:167:VAL:HG23 | 31:BE:170:LEU:CD1 | 2.28                     | 0.62              |
| 31:BE:21:VAL:HG23  | 31:BE:21:VAL:O    | 1.98                     | 0.62              |
| 34:BH:10:PRO:HG3   | 34:BH:50:VAL:C    | 2.18                     | 0.62              |
| 35:BI:3:VAL:CA     | 35:BI:39:ALA:HB2  | 2.28                     | 0.62              |
| 27:BA:2875:C:O2'   | 42:BT:5:ALA:HB3   | 1.99                     | 0.62              |
| 44:BV:6:LYS:HG2    | 44:BV:10:LYS:O    | 1.99                     | 0.62              |
| 1:CA:1445:C:C2'    | 1:CA:1446:U:H5'   | 2.29                     | 0.62              |
| 1:CA:237:C:H5''    | 17:CQ:25:ARG:HH11 | 1.61                     | 0.62              |
| 4:CD:158:ILE:HG22  | 4:CD:162:LEU:HD12 | 1.81                     | 0.62              |
| 11:CK:104:GLN:HG2  | 11:CK:105:VAL:N   | 2.14                     | 0.62              |
| 27:DA:1336:A:H2'   | 27:DA:1337:G:C8   | 2.34                     | 0.62              |
| 27:DA:1973:G:H2'   | 27:DA:1974:C:H6   | 1.59                     | 0.62              |
| 27:DA:2232:U:O2'   | 27:DA:2233:U:H5'  | 1.99                     | 0.62              |
| 27:DA:415:A:H2'    | 27:DA:416:C:H6    | 1.63                     | 0.62              |
| 27:DA:61:G:HO2'    | 27:DA:62:C:H6     | 1.47                     | 0.62              |
| 27:DA:999:U:H2'    | 27:DA:1000:A:C5'  | 2.27                     | 0.62              |
| 30:DD:208:LYS:HG2  | 30:DD:210:GLY:O   | 1.99                     | 0.62              |
| 30:DD:68:LYS:O     | 30:DD:68:LYS:HG3  | 1.99                     | 0.62              |
| 33:DG:39:ILE:HD13  | 33:DG:157:ILE:CG2 | 2.29                     | 0.62              |
| 33:DG:25:TYR:CE2   | 33:DG:31:VAL:HG23 | 2.34                     | 0.62              |
| 33:DG:81:LYS:O     | 33:DG:82:LEU:O    | 2.16                     | 0.62              |
| 34:DH:84:SER:O     | 34:DH:85:LYS:HB3  | 1.98                     | 0.62              |
| 36:DN:4:TYR:CD1    | 36:DN:4:TYR:N     | 2.67                     | 0.62              |
| 38:DP:47:ASP:HB3   | 38:DP:48:PRO:HA   | 1.79                     | 0.62              |
| 38:DP:66:GLY:O     | 38:DP:67:MET:HB3  | 1.97                     | 0.62              |
| 42:DT:3:ARG:O      | 42:DT:5:ALA:N     | 2.32                     | 0.62              |
| 42:DT:93:ARG:HG3   | 42:DT:93:ARG:HH11 | 1.63                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:DT:92:GLY:C    | 42:DT:94:ALA:H     | 2.02                     | 0.62              |
| 43:DU:42:ALA:C    | 43:DU:44:ASN:H     | 2.01                     | 0.62              |
| 48:DZ:93:GLU:HB2  | 48:DZ:95:VAL:HG23  | 1.79                     | 0.62              |
| 1:AA:271:C:H2'    | 1:AA:272:C:H6      | 1.60                     | 0.62              |
| 19:AS:29:ARG:O    | 19:AS:31:ILE:HG22  | 1.99                     | 0.62              |
| 58:B9:24:TYR:CE2  | 58:B9:35:ARG:HD2   | 2.34                     | 0.62              |
| 27:BA:1850:G:H2'  | 27:BA:1851:U:C6    | 2.34                     | 0.62              |
| 27:BA:2144:U:H4'  | 27:BA:2145:C:H5    | 1.64                     | 0.62              |
| 27:BA:2171:A:H4'  | 27:BA:2172:U:H5'   | 1.78                     | 0.62              |
| 27:BA:2698:U:H2'  | 27:BA:2699:C:C6    | 2.34                     | 0.62              |
| 27:BA:556:G:H2'   | 27:BA:557:U:C6     | 2.34                     | 0.62              |
| 27:BA:826:U:H5''  | 27:BA:826:U:H6     | 1.62                     | 0.62              |
| 29:BC:86:ALA:HB2  | 29:BC:152:ILE:CB   | 2.29                     | 0.62              |
| 30:BD:31:LYS:HE3  | 30:BD:33:LEU:CD2   | 2.25                     | 0.62              |
| 31:BE:69:LYS:C    | 31:BE:71:GLY:N     | 2.52                     | 0.62              |
| 35:BI:7:GLU:HG3   | 35:BI:7:GLU:O      | 1.99                     | 0.62              |
| 36:BN:5:VAL:HG13  | 36:BN:5:VAL:O      | 1.98                     | 0.62              |
| 43:BU:104:GLN:C   | 43:BU:104:GLN:HE21 | 2.02                     | 0.62              |
| 1:CA:1187:G:H2'   | 1:CA:1188:A:C8     | 2.33                     | 0.62              |
| 1:CA:1492:A:H3'   | 26:CZ:6:5OH:HNP    | 1.64                     | 0.62              |
| 1:CA:402:G:O2'    | 1:CA:403:C:H5'     | 1.99                     | 0.62              |
| 1:CA:817:C:C1'    | 1:CA:819:A:H5'     | 2.28                     | 0.62              |
| 1:CA:956:U:O2'    | 1:CA:957:U:H5'     | 1.99                     | 0.62              |
| 1:CA:96:U:H2'     | 1:CA:97:G:C8       | 2.33                     | 0.62              |
| 7:CG:65:ALA:CB    | 7:CG:124:LEU:HD23  | 2.29                     | 0.62              |
| 1:CA:472:A:H5''   | 16:CP:80:PHE:HB3   | 1.81                     | 0.62              |
| 55:D6:17:LYS:HB3  | 55:D6:18:ARG:NH1   | 2.14                     | 0.62              |
| 27:DA:1329:U:H5'  | 27:DA:1330:C:H5    | 1.62                     | 0.62              |
| 27:DA:1877:A:H5'  | 27:DA:1878:G:OP2   | 1.99                     | 0.62              |
| 27:DA:2174:C:O2'  | 27:DA:2175:C:O4'   | 2.16                     | 0.62              |
| 27:DA:2068:U:H3   | 27:DA:2430:A:H2    | 1.47                     | 0.62              |
| 27:DA:2560:C:H42  | 27:DA:2561:A:N6    | 1.95                     | 0.62              |
| 27:DA:1629:U:H1'  | 27:DA:2698:U:H5''  | 1.79                     | 0.62              |
| 27:DA:702:G:H1    | 27:DA:730:C:H42    | 1.48                     | 0.62              |
| 29:DC:41:VAL:HG12 | 29:DC:213:TYR:HA   | 1.81                     | 0.62              |
| 37:DO:87:ILE:HG12 | 37:DO:93:PRO:HA    | 1.81                     | 0.62              |
| 41:DS:13:ARG:O    | 41:DS:14:VAL:HB    | 1.98                     | 0.62              |
| 48:DZ:119:ILE:HB  | 48:DZ:170:ILE:C    | 2.20                     | 0.62              |
| 1:AA:1472:U:O2'   | 1:AA:1473:A:H5'    | 1.99                     | 0.62              |
| 1:AA:627:G:H2'    | 1:AA:628:G:C8      | 2.31                     | 0.62              |
| 2:AB:197:VAL:HB   | 2:AB:200:ILE:CG1   | 2.29                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:26:PHE:CD1    | 5:AE:26:PHE:N      | 2.66                     | 0.62              |
| 6:AF:5:GLU:HG3     | 6:AF:93:SER:OG     | 1.99                     | 0.62              |
| 5:AE:80:ILE:CG2    | 8:AH:104:ARG:HH12  | 2.11                     | 0.62              |
| 8:AH:25:ASP:HA     | 8:AH:59:LEU:O      | 1.99                     | 0.62              |
| 9:AI:115:GLY:C     | 9:AI:116:LYS:HG2   | 2.19                     | 0.62              |
| 12:AL:31:ARG:HH21  | 12:AL:58:THR:HG21  | 1.64                     | 0.62              |
| 18:AR:37:VAL:HG23  | 18:AR:38:GLU:N     | 2.14                     | 0.62              |
| 27:BA:2271:G:H5'   | 49:B0:20:ARG:HG2   | 1.81                     | 0.62              |
| 46:BX:5:TYR:CZ     | 51:B2:30:ARG:HB2   | 2.34                     | 0.62              |
| 27:BA:1192:G:C2'   | 27:BA:1193:G:C5'   | 2.78                     | 0.62              |
| 27:BA:1346:G:C4    | 27:BA:1347:G:C8    | 2.88                     | 0.62              |
| 27:BA:142(A):C:O2' | 27:BA:143:G:H5'    | 1.98                     | 0.62              |
| 27:BA:1494:A:O2'   | 27:BA:1495:A:H5''  | 1.98                     | 0.62              |
| 27:BA:1596:A:O2'   | 27:BA:1597:A:H5'   | 2.00                     | 0.62              |
| 27:BA:1722:A:C6    | 27:BA:1740:G:H8    | 2.16                     | 0.62              |
| 27:BA:1848:A:O2'   | 27:BA:1849:G:H8    | 1.82                     | 0.62              |
| 27:BA:1850:G:H2'   | 27:BA:1851:U:H6    | 1.64                     | 0.62              |
| 27:BA:271(F):C:N4  | 27:BA:271(R):G:H1  | 1.93                     | 0.62              |
| 27:BA:485:C:H2'    | 27:BA:486:C:H6     | 1.62                     | 0.62              |
| 31:BE:179:GLU:HB3  | 31:BE:181:LEU:HD22 | 1.80                     | 0.62              |
| 33:BG:43:LEU:HB2   | 33:BG:88:ILE:HD11  | 1.81                     | 0.62              |
| 35:BI:28:ASN:N     | 35:BI:28:ASN:HD22  | 1.97                     | 0.62              |
| 40:BR:9:LYS:C      | 40:BR:10:LEU:HG    | 2.18                     | 0.62              |
| 42:BT:32:TYR:CD2   | 42:BT:32:TYR:N     | 2.67                     | 0.62              |
| 1:CA:1457:G:H2'    | 1:CA:1458:G:H8     | 1.65                     | 0.62              |
| 1:CA:250:A:H2      | 1:CA:274:A:H61     | 1.44                     | 0.62              |
| 1:CA:935:A:H2      | 1:CA:1383:C:N4     | 1.95                     | 0.62              |
| 1:CA:939:G:C5'     | 7:CG:102:ARG:HH12  | 2.12                     | 0.62              |
| 1:CA:939:G:C5'     | 7:CG:102:ARG:HH22  | 2.11                     | 0.62              |
| 2:CB:11:LEU:CD1    | 2:CB:217:ARG:NH2   | 2.61                     | 0.62              |
| 5:CE:62:ALA:O      | 5:CE:65:ASN:N      | 2.30                     | 0.62              |
| 12:CL:24:LEU:HG    | 12:CL:59:SER:OG    | 2.00                     | 0.62              |
| 13:CM:112:GLY:O    | 13:CM:113:PRO:O    | 2.17                     | 0.62              |
| 27:DA:107:C:O2'    | 27:DA:108:U:H5'    | 2.00                     | 0.62              |
| 27:DA:2416:C:H2'   | 27:DA:2417:C:H6    | 1.63                     | 0.62              |
| 27:DA:2052:G:H22   | 27:DA:2618:G:H1'   | 1.64                     | 0.62              |
| 27:DA:2869:G:H2'   | 27:DA:2870:C:C6    | 2.34                     | 0.62              |
| 27:DA:579:G:H2'    | 27:DA:580:C:H6     | 1.58                     | 0.62              |
| 27:DA:597:U:H2'    | 27:DA:598:G:H8     | 1.62                     | 0.62              |
| 27:DA:848:G:H5'    | 27:DA:848:G:H8     | 1.64                     | 0.62              |
| 27:DA:868:U:H3     | 27:DA:912:C:H1'    | 1.63                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:941:A:H2'   | 27:DA:942:G:C8     | 2.34                     | 0.62              |
| 27:DA:999:U:H5''  | 27:DA:1154:G:O6    | 1.99                     | 0.62              |
| 28:DB:27:C:H5''   | 28:DB:27:C:H6      | 1.64                     | 0.62              |
| 32:DF:158:THR:HB  | 32:DF:195:ASP:OD2  | 1.98                     | 0.62              |
| 32:DF:57:VAL:HG12 | 32:DF:59:TYR:HD1   | 1.63                     | 0.62              |
| 38:DP:115:LEU:CD2 | 38:DP:115:LEU:N    | 2.62                     | 0.62              |
| 27:DA:908:C:H3'   | 39:DQ:22:LYS:HZ2   | 1.60                     | 0.62              |
| 39:DQ:108:GLY:HA3 | 48:DZ:115:VAL:HG11 | 1.80                     | 0.62              |
| 6:AF:77:ARG:O     | 6:AF:79:LEU:N      | 2.33                     | 0.62              |
| 6:AF:81:ILE:HG22  | 6:AF:81:ILE:O      | 1.99                     | 0.62              |
| 11:AK:96:ARG:O    | 11:AK:99:GLN:HB2   | 2.00                     | 0.62              |
| 55:B6:51:GLU:O    | 55:B6:52:VAL:HB    | 2.00                     | 0.62              |
| 27:BA:1051:G:HO2' | 27:BA:1052:C:H6    | 1.47                     | 0.62              |
| 27:BA:1547:C:H2'  | 27:BA:1548:C:C6    | 2.34                     | 0.62              |
| 27:BA:1605:C:O2'  | 27:BA:1606:G:H5'   | 2.00                     | 0.62              |
| 27:BA:1947:C:H6   | 27:BA:1947:C:H5''  | 1.64                     | 0.62              |
| 27:BA:216:A:H2'   | 27:BA:217:G:C8     | 2.34                     | 0.62              |
| 27:BA:297:C:H2'   | 27:BA:298:G:O4'    | 2.00                     | 0.62              |
| 27:BA:58:G:N2     | 27:BA:70:G:C4      | 2.67                     | 0.62              |
| 27:BA:635:C:O2'   | 27:BA:636:G:H5'    | 2.00                     | 0.62              |
| 27:BA:670:A:C8    | 27:BA:670:A:O5'    | 2.52                     | 0.62              |
| 30:BD:52:ARG:HH12 | 30:BD:249:PRO:HG2  | 1.65                     | 0.62              |
| 30:BD:28:GLU:HB2  | 30:BD:29:PRO:HD3   | 1.80                     | 0.62              |
| 31:BE:70:ALA:O    | 31:BE:71:GLY:C     | 2.36                     | 0.62              |
| 33:BG:102:PHE:HA  | 33:BG:105:LYS:HZ1  | 1.63                     | 0.62              |
| 40:BR:56:LYS:C    | 40:BR:57:ARG:O     | 2.32                     | 0.62              |
| 45:BW:90:ARG:NH1  | 45:BW:90:ARG:CG    | 2.58                     | 0.62              |
| 47:BY:31:LEU:CB   | 47:BY:32:PRO:CA    | 2.78                     | 0.62              |
| 48:BZ:8:TYR:HE2   | 48:BZ:34:ARG:HD2   | 1.62                     | 0.62              |
| 1:CA:749:C:O2'    | 1:CA:750:G:H5'     | 1.99                     | 0.62              |
| 1:CA:814:A:O2'    | 1:CA:815:A:H5''    | 1.99                     | 0.62              |
| 3:CC:12:LEU:O     | 3:CC:16:ARG:O      | 2.18                     | 0.62              |
| 9:CI:19:LEU:C     | 9:CI:20:ARG:HD2    | 2.20                     | 0.62              |
| 16:CP:21:VAL:O    | 16:CP:21:VAL:HG13  | 1.99                     | 0.62              |
| 51:D2:10:LEU:HD21 | 51:D2:59:ARG:HD2   | 1.81                     | 0.62              |
| 27:DA:1600:C:O2'  | 27:DA:1601:G:H5'   | 1.99                     | 0.62              |
| 27:DA:1688:U:H1'  | 27:DA:1701:A:N6    | 2.15                     | 0.62              |
| 27:DA:1849:G:C2   | 27:DA:1850:G:C8    | 2.88                     | 0.62              |
| 27:DA:813:U:H3    | 27:DA:1194:A:H61   | 1.46                     | 0.62              |
| 28:DB:15:A:H1'    | 28:DB:110:G:C5     | 2.35                     | 0.62              |
| 31:DE:79:ARG:NH1  | 31:DE:195:LEU:HD23 | 2.14                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:DO:12:ASP:HB3   | 37:DO:85:VAL:HG22 | 1.81                     | 0.62              |
| 41:DS:97:ARG:HH12  | 41:DS:99:LYS:CG   | 2.11                     | 0.62              |
| 43:DU:9:VAL:O      | 43:DU:12:ARG:HB2  | 1.99                     | 0.62              |
| 45:DW:15:ARG:CZ    | 54:D5:20:ARG:NH2  | 2.62                     | 0.62              |
| 45:DW:18:ARG:HG2   | 45:DW:18:ARG:HH11 | 1.63                     | 0.62              |
| 27:DA:486:C:H4'    | 45:DW:60:ASN:OD1  | 1.99                     | 0.62              |
| 1:AA:1423:G:O2'    | 1:AA:1424:C:H5'   | 1.99                     | 0.62              |
| 1:AA:179:A:H2'     | 1:AA:180:U:H6     | 1.64                     | 0.62              |
| 1:AA:327:A:HO2'    | 1:AA:329:A:H8     | 1.45                     | 0.62              |
| 1:AA:959:A:H2'     | 1:AA:960:U:H4'    | 1.82                     | 0.62              |
| 14:AN:51:GLY:O     | 14:AN:53:LEU:N    | 2.33                     | 0.62              |
| 23:AW:52:G:O2'     | 23:AW:53:U:H5'    | 1.99                     | 0.62              |
| 51:B2:53:LEU:HD22  | 51:B2:57:ILE:CD1  | 2.30                     | 0.62              |
| 52:B3:8:LEU:CD1    | 52:B3:31:LEU:HD23 | 2.28                     | 0.62              |
| 27:BA:2014:A:H2'   | 27:BA:2015:A:C8   | 2.34                     | 0.62              |
| 27:BA:339:U:H6     | 27:BA:339:U:O5'   | 1.82                     | 0.62              |
| 28:BB:35:U:H2'     | 28:BB:36:C:H6     | 1.64                     | 0.62              |
| 32:BF:206:ILE:HG13 | 32:BF:206:ILE:O   | 1.98                     | 0.62              |
| 34:BH:43:VAL:HG11  | 34:BH:52:VAL:HA   | 1.80                     | 0.62              |
| 35:BI:10:GLU:O     | 35:BI:11:ASN:CB   | 2.47                     | 0.62              |
| 27:BA:2039:C:OP2   | 36:BN:109:LYS:HD3 | 2.00                     | 0.62              |
| 36:BN:63:THR:HG22  | 36:BN:64:GLY:N    | 2.08                     | 0.62              |
| 36:BN:68:GLU:OE1   | 36:BN:68:GLU:HA   | 1.98                     | 0.62              |
| 39:BQ:39:PRO:HG3   | 39:BQ:99:PRO:HD3  | 1.81                     | 0.62              |
| 41:BS:87:PHE:HD2   | 41:BS:88:ASP:H    | 1.46                     | 0.62              |
| 48:BZ:71:ARG:HG2   | 48:BZ:88:PHE:HB2  | 1.81                     | 0.62              |
| 1:CA:341:C:H2'     | 1:CA:342:C:C6     | 2.34                     | 0.62              |
| 2:CB:56:ARG:HH11   | 2:CB:56:ARG:HG2   | 1.64                     | 0.62              |
| 9:CI:28:VAL:HA     | 9:CI:63:ILE:O     | 1.99                     | 0.62              |
| 21:CU:10:ARG:HA    | 21:CU:13:ILE:HD12 | 1.82                     | 0.62              |
| 27:DA:1322:A:O2'   | 27:DA:1323:U:H5'  | 2.00                     | 0.62              |
| 27:DA:1452:A:C6    | 27:DA:2702:U:H1'  | 2.34                     | 0.62              |
| 27:DA:1669:A:H5''  | 27:DA:2550:G:OP1  | 1.98                     | 0.62              |
| 27:DA:1854:A:H62   | 27:DA:1888:G:H8   | 1.47                     | 0.62              |
| 27:DA:51:G:N3      | 27:DA:119:A:C2    | 2.68                     | 0.62              |
| 27:DA:601:C:OP1    | 32:DF:108:LYS:NZ  | 2.24                     | 0.62              |
| 27:DA:90:U:O2'     | 27:DA:92:A:C5'    | 2.40                     | 0.62              |
| 30:DD:176:ARG:HH11 | 30:DD:176:ARG:HG2 | 1.63                     | 0.62              |
| 32:DF:116:ASP:O    | 32:DF:119:ARG:N   | 2.32                     | 0.62              |
| 33:DG:124:SER:HB2  | 33:DG:131:TYR:CE1 | 2.35                     | 0.62              |
| 33:DG:85:GLY:C     | 33:DG:87:PRO:HD2  | 2.19                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DH:92:ILE:O    | 34:DH:94:TYR:N     | 2.32                     | 0.62              |
| 38:DP:50:ARG:HH21 | 38:DP:50:ARG:HG2   | 1.62                     | 0.62              |
| 43:DU:25:TRP:CG   | 43:DU:26:GLY:N     | 2.67                     | 0.62              |
| 44:DV:19:LYS:CE   | 44:DV:20:LEU:H     | 2.12                     | 0.62              |
| 45:DW:65:LEU:HD22 | 45:DW:68:ARG:H     | 1.64                     | 0.62              |
| 48:DZ:91:SER:HB3  | 48:DZ:93:GLU:HG2   | 1.79                     | 0.62              |
| 1:AA:1207:G:H2'   | 1:AA:1208:C:H6     | 1.62                     | 0.62              |
| 1:AA:1321:C:C3'   | 1:AA:1322:C:H5''   | 2.29                     | 0.62              |
| 11:AK:78:GLN:O    | 11:AK:103:LEU:HD13 | 1.99                     | 0.62              |
| 13:AM:4:ILE:HG12  | 13:AM:57:ARG:HG3   | 1.80                     | 0.62              |
| 15:AO:39:LEU:HD12 | 15:AO:56:LEU:HB2   | 1.82                     | 0.62              |
| 18:AR:36:ASN:ND2  | 18:AR:39:VAL:HG21  | 2.15                     | 0.62              |
| 18:AR:53:ARG:HG2  | 18:AR:53:ARG:HH11  | 1.65                     | 0.62              |
| 27:BA:1310:G:N2   | 27:BA:1313:U:C5    | 2.67                     | 0.62              |
| 27:BA:147:U:H2'   | 27:BA:148:C:C6     | 2.35                     | 0.62              |
| 27:BA:2680:C:O2'  | 27:BA:2681:C:H5'   | 1.99                     | 0.62              |
| 36:BN:30:ILE:O    | 36:BN:34:LEU:HD22  | 2.00                     | 0.62              |
| 37:BO:63:VAL:HB   | 37:BO:102:VAL:HG12 | 1.82                     | 0.62              |
| 27:BA:942:G:OP1   | 38:BP:41:ARG:NH2   | 2.33                     | 0.62              |
| 46:BX:59:VAL:O    | 46:BX:59:VAL:HG12  | 1.98                     | 0.62              |
| 1:CA:102:G:H2'    | 1:CA:103:C:H6      | 1.64                     | 0.62              |
| 1:CA:1458:G:OP1   | 20:CT:35:THR:HG21  | 2.00                     | 0.62              |
| 1:CA:1510:U:H2'   | 1:CA:1511:G:C8     | 2.34                     | 0.62              |
| 1:CA:652:U:O2'    | 1:CA:653:A:C5'     | 2.45                     | 0.62              |
| 2:CB:19:HIS:ND1   | 2:CB:189:ASP:OD2   | 2.31                     | 0.62              |
| 2:CB:76:GLN:O     | 2:CB:77:ALA:HB2    | 1.99                     | 0.62              |
| 5:CE:86:ALA:HB3   | 5:CE:130:ASN:HD22  | 1.65                     | 0.62              |
| 8:CH:68:ARG:HG2   | 8:CH:68:ARG:NH1    | 2.14                     | 0.62              |
| 9:CI:56:LEU:HD23  | 9:CI:56:LEU:O      | 1.99                     | 0.62              |
| 1:CA:973:G:C1'    | 10:CJ:55:LYS:HE2   | 2.28                     | 0.62              |
| 11:CK:29:ILE:HD13 | 11:CK:44:SER:HB3   | 1.81                     | 0.62              |
| 17:CQ:31:LEU:HD23 | 17:CQ:32:TYR:OH    | 2.00                     | 0.62              |
| 25:CY:27:C:N4     | 25:CY:41:G:H1      | 1.97                     | 0.62              |
| 27:DA:1277:G:O2'  | 40:DR:24:GLN:HG2   | 1.99                     | 0.62              |
| 27:DA:2371:G:O2'  | 55:D6:46:HIS:CE1   | 2.52                     | 0.62              |
| 27:DA:2509:G:H2'  | 27:DA:2510:C:C6    | 2.34                     | 0.62              |
| 27:DA:2762:G:H5'  | 27:DA:2763:G:OP2   | 1.99                     | 0.62              |
| 30:DD:211:ARG:HA  | 30:DD:214:TRP:CD2  | 2.35                     | 0.62              |
| 31:DE:13:ARG:HB3  | 31:DE:22:PRO:HA    | 1.82                     | 0.62              |
| 32:DF:23:ASP:O    | 32:DF:24:LEU:HD22  | 1.99                     | 0.62              |
| 33:DG:131:TYR:CE2 | 33:DG:133:LEU:HD23 | 2.34                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DG:72:ARG:NH1  | 33:DG:86:MET:HG2  | 2.15                     | 0.62              |
| 34:DH:137:ASP:HB3 | 34:DH:140:LYS:HB3 | 1.81                     | 0.62              |
| 36:DN:16:ILE:HG23 | 36:DN:54:VAL:CG2  | 2.29                     | 0.62              |
| 37:DO:13:ASN:C    | 37:DO:15:GLY:H    | 2.02                     | 0.62              |
| 40:DR:73:VAL:O    | 40:DR:76:VAL:HB   | 2.00                     | 0.62              |
| 48:DZ:27:MET:CE   | 48:DZ:32:LEU:HD11 | 2.30                     | 0.62              |
| 1:AA:1321:C:H5''  | 1:AA:1322:C:H2'   | 1.81                     | 0.62              |
| 1:AA:232:G:O2'    | 1:AA:233:C:H5'    | 2.00                     | 0.62              |
| 1:AA:942:G:H2'    | 1:AA:942:G:N3     | 2.13                     | 0.62              |
| 3:AC:103:VAL:HG12 | 3:AC:103:VAL:O    | 1.99                     | 0.62              |
| 7:AG:27:ILE:HG23  | 7:AG:39:ALA:O     | 2.00                     | 0.62              |
| 9:AI:53:VAL:HG11  | 9:AI:85:LEU:HD22  | 1.82                     | 0.62              |
| 11:AK:51:LYS:HA   | 11:AK:55:LYS:HD3  | 1.81                     | 0.62              |
| 13:AM:40:ASN:ND2  | 13:AM:42:ALA:HB3  | 2.14                     | 0.62              |
| 13:AM:84:ILE:HB   | 19:AS:66:MET:HE1  | 1.82                     | 0.62              |
| 23:AW:42:G:C3'    | 23:AW:43:C:H5''   | 2.30                     | 0.62              |
| 27:BA:1686:C:H5'  | 27:BA:1686:C:C6   | 2.33                     | 0.62              |
| 27:BA:2317:C:O2'  | 27:BA:2318:G:H5'  | 1.99                     | 0.62              |
| 27:BA:2472:G:C5'  | 27:BA:2473:U:H5'' | 2.29                     | 0.62              |
| 27:BA:2533:A:C2'  | 27:BA:2534:A:H5'' | 2.30                     | 0.62              |
| 30:BD:261:LYS:HE2 | 30:BD:263:ARG:NH2 | 2.15                     | 0.62              |
| 32:BF:108:LYS:O   | 32:BF:112:MET:HB2 | 1.99                     | 0.62              |
| 32:BF:20:LEU:HB3  | 32:BF:23:ASP:OD2  | 1.99                     | 0.62              |
| 32:BF:68:LYS:C    | 32:BF:70:THR:H    | 2.02                     | 0.62              |
| 34:BH:10:PRO:HG2  | 34:BH:10:PRO:O    | 2.00                     | 0.62              |
| 34:BH:99:VAL:O    | 34:BH:99:VAL:HG12 | 1.99                     | 0.62              |
| 38:BP:13:ASN:HD22 | 38:BP:13:ASN:C    | 2.03                     | 0.62              |
| 43:BU:24:TYR:CE1  | 43:BU:38:THR:HG21 | 2.34                     | 0.62              |
| 47:BY:96:ILE:CG2  | 47:BY:97:ARG:H    | 2.12                     | 0.62              |
| 1:CA:1275:A:H2'   | 1:CA:1276:G:H8    | 1.64                     | 0.62              |
| 1:CA:419:C:C2'    | 1:CA:420:U:H5'    | 2.30                     | 0.62              |
| 1:CA:527:G:C2'    | 1:CA:528:C:H5'    | 2.29                     | 0.62              |
| 4:CD:36:ARG:O     | 4:CD:38:TYR:N     | 2.31                     | 0.62              |
| 1:CA:5:U:H2'      | 4:CD:86:LYS:HE2   | 1.80                     | 0.62              |
| 7:CG:102:ARG:O    | 7:CG:106:GLN:HG2  | 1.98                     | 0.62              |
| 7:CG:85:TYR:CD1   | 7:CG:154:TYR:CE1  | 2.80                     | 0.62              |
| 12:CL:86:ARG:HA   | 12:CL:94:ARG:HA   | 1.81                     | 0.62              |
| 13:CM:4:ILE:HG22  | 13:CM:5:ALA:N     | 2.10                     | 0.62              |
| 15:CO:35:ARG:NH2  | 15:CO:59:MET:HE2  | 2.06                     | 0.62              |
| 20:CT:48:LYS:O    | 20:CT:49:ALA:CB   | 2.47                     | 0.62              |
| 27:DA:125:G:H21   | 56:D7:48:LYS:CE   | 2.11                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:1693:U:H4'  | 27:DA:1694:C:OP2  | 1.98                     | 0.62              |
| 27:DA:2126:A:H4'  | 27:DA:2127:G:O5'  | 1.99                     | 0.62              |
| 27:DA:594:U:H3    | 27:DA:663:G:H1    | 1.47                     | 0.62              |
| 27:DA:748:G:C5'   | 45:DW:89:ALA:HB2  | 2.27                     | 0.62              |
| 27:DA:960:A:N7    | 27:DA:962:G:C4    | 2.68                     | 0.62              |
| 29:DC:39:GLU:OE2  | 29:DC:68:LEU:HD22 | 2.00                     | 0.62              |
| 32:DF:11:VAL:HG12 | 32:DF:12:LEU:HG   | 1.79                     | 0.62              |
| 33:DG:125:PHE:HA  | 33:DG:131:TYR:HA  | 1.82                     | 0.62              |
| 33:DG:63:ILE:HA   | 33:DG:143:GLU:CG  | 2.30                     | 0.62              |
| 46:DX:57:LEU:HD11 | 46:DX:78:LYS:CD   | 2.29                     | 0.62              |
| 1:AA:36:C:C5'     | 12:AL:119:THR:O   | 2.48                     | 0.62              |
| 1:AA:909:A:C2'    | 1:AA:910:C:H5'    | 2.29                     | 0.62              |
| 2:AB:57:PHE:HD2   | 2:AB:185:ILE:HD11 | 1.64                     | 0.62              |
| 3:AC:14:ILE:HD13  | 3:AC:178:LEU:HB3  | 1.80                     | 0.62              |
| 4:AD:199:ASN:HB3  | 4:AD:202:LEU:HD12 | 1.81                     | 0.62              |
| 5:AE:43:LEU:CD2   | 5:AE:132:ALA:HB1  | 2.30                     | 0.62              |
| 11:AK:125:PHE:N   | 11:AK:125:PHE:CD1 | 2.62                     | 0.62              |
| 1:AA:664:G:P      | 18:AR:64:ARG:HH21 | 2.22                     | 0.62              |
| 6:AF:89:MET:SD    | 18:AR:76:LEU:HD21 | 2.39                     | 0.62              |
| 24:AX:73:A:H5'    | 24:AX:74:C:H5'    | 1.82                     | 0.62              |
| 55:B6:15:GLU:O    | 55:B6:15:GLU:HG2  | 2.00                     | 0.62              |
| 27:BA:1332:G:H22  | 27:BA:1609:A:C2'  | 2.12                     | 0.62              |
| 27:BA:529:A:H62   | 27:BA:2041:U:H3   | 1.45                     | 0.62              |
| 27:BA:2511:U:O2'  | 27:BA:2512:C:H5'  | 2.00                     | 0.62              |
| 27:BA:542:C:N4    | 27:BA:543:C:H41   | 1.98                     | 0.62              |
| 27:BA:722:A:H5'   | 27:BA:723:G:OP2   | 2.00                     | 0.62              |
| 28:BB:42:C:H5'    | 33:BG:68:PRO:O    | 2.00                     | 0.62              |
| 36:BN:62:VAL:HG11 | 36:BN:67:LEU:CD2  | 2.30                     | 0.62              |
| 37:BO:17:ARG:HE   | 37:BO:47:ILE:HD13 | 1.65                     | 0.62              |
| 41:BS:17:ARG:CZ   | 41:BS:25:ARG:HH21 | 2.12                     | 0.62              |
| 42:BT:38:ASN:O    | 42:BT:38:ASN:ND2  | 2.33                     | 0.62              |
| 27:BA:1754:C:O5'  | 42:BT:96:ARG:NH1  | 2.32                     | 0.62              |
| 45:BW:90:ARG:HG3  | 45:BW:90:ARG:NH1  | 2.14                     | 0.62              |
| 1:CA:1158:C:H2'   | 1:CA:1158:C:O2    | 1.99                     | 0.62              |
| 1:CA:1320:C:C2    | 19:CS:72:GLY:HA3  | 2.34                     | 0.62              |
| 1:CA:542:G:H2'    | 1:CA:543:C:C6     | 2.34                     | 0.62              |
| 1:CA:552:U:H4'    | 12:CL:83:ARG:HG2  | 1.80                     | 0.62              |
| 1:CA:554:C:H2'    | 1:CA:555:C:H6     | 1.64                     | 0.62              |
| 1:CA:870:U:H4'    | 1:CA:871:U:O5'    | 1.99                     | 0.62              |
| 1:CA:940:C:H2'    | 1:CA:941:G:C8     | 2.35                     | 0.62              |
| 6:CF:9:VAL:HB     | 6:CF:87:ARG:HB2   | 1.81                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:CH:111:ILE:HG22  | 8:CH:112:LEU:N    | 2.14                     | 0.62              |
| 9:CI:79:LEU:HD21   | 9:CI:102:LEU:HA   | 1.81                     | 0.62              |
| 9:CI:83:ARG:HH21   | 9:CI:102:LEU:HD11 | 1.64                     | 0.62              |
| 13:CM:94:ARG:O     | 13:CM:95:GLY:O    | 2.17                     | 0.62              |
| 53:D4:46:ASN:ND2   | 53:D4:47:VAL:N    | 2.48                     | 0.62              |
| 27:DA:1236:G:O2'   | 27:DA:1237:A:OP2  | 2.15                     | 0.62              |
| 27:DA:157:U:OP1    | 27:DA:157:U:H6    | 1.83                     | 0.62              |
| 27:DA:1782:C:O2'   | 27:DA:1783:A:H5'  | 1.99                     | 0.62              |
| 27:DA:1825:A:H2'   | 27:DA:1826:G:C8   | 2.35                     | 0.62              |
| 27:DA:2123:G:H2'   | 27:DA:2124:G:H8   | 1.64                     | 0.62              |
| 27:DA:246:C:C2'    | 27:DA:247:G:H5'   | 2.29                     | 0.62              |
| 27:DA:577:G:H2'    | 27:DA:578:A:O4'   | 2.00                     | 0.62              |
| 27:DA:930:U:OP1    | 27:DA:930:U:H3'   | 1.98                     | 0.62              |
| 30:DD:147:LEU:H    | 30:DD:154:LYS:HG3 | 1.65                     | 0.62              |
| 37:DO:104:ARG:NH2  | 42:DT:33:LYS:HE2  | 2.15                     | 0.62              |
| 37:DO:97:ARG:HE    | 37:DO:99:PHE:HE1  | 1.45                     | 0.62              |
| 27:DA:911:A:H2'    | 39:DQ:9:TYR:CZ    | 2.34                     | 0.62              |
| 44:DV:2:PHE:CE1    | 44:DV:13:ARG:NH1  | 2.68                     | 0.62              |
| 46:DX:36:LYS:HE2   | 46:DX:55:ASN:HA   | 1.80                     | 0.62              |
| 1:AA:1252:A:H2'    | 1:AA:1253:G:O4'   | 2.00                     | 0.62              |
| 1:AA:632:A:H2'     | 1:AA:633:G:O4'    | 2.00                     | 0.62              |
| 11:AK:57:THR:CG2   | 11:AK:58:PRO:HD2  | 2.30                     | 0.62              |
| 3:AC:6:HIS:CG      | 14:AN:49:HIS:HB3  | 2.34                     | 0.62              |
| 20:AT:41:ILE:O     | 20:AT:44:ALA:HB3  | 2.00                     | 0.62              |
| 25:AY:30:A:H2'     | 25:AY:31:U:C6     | 2.33                     | 0.62              |
| 27:BA:2353:G:H1'   | 49:B0:34:GLY:HA3  | 1.79                     | 0.62              |
| 58:B9:18:ARG:HH12  | 58:B9:21:GLY:HA2  | 1.63                     | 0.62              |
| 27:BA:1054:A:N3    | 27:BA:1055:G:N7   | 2.48                     | 0.62              |
| 27:BA:1621:U:H5''  | 27:BA:1622:G:OP1  | 2.00                     | 0.62              |
| 27:BA:1777:U:H2'   | 27:BA:1778:U:C6   | 2.35                     | 0.62              |
| 27:BA:1844:C:O2'   | 27:BA:1845:G:H5'  | 2.00                     | 0.62              |
| 27:BA:1934:C:O2'   | 27:BA:1935:G:H5'  | 1.99                     | 0.62              |
| 27:BA:225:A:O2'    | 27:BA:257:A:H4'   | 2.00                     | 0.62              |
| 27:BA:2387:U:H6    | 27:BA:2387:U:OP2  | 1.82                     | 0.62              |
| 27:BA:1462:C:H4'   | 27:BA:2703:C:H5'  | 1.80                     | 0.62              |
| 27:BA:2756:U:H1'   | 27:BA:2757:A:H5'' | 1.81                     | 0.62              |
| 27:BA:44:G:H5''    | 27:BA:45:C:OP1    | 1.98                     | 0.62              |
| 30:BD:197:GLY:O    | 30:BD:198:ASN:HB3 | 2.00                     | 0.62              |
| 30:BD:33:LEU:CD1   | 30:BD:33:LEU:H    | 2.13                     | 0.62              |
| 32:BF:21:ALA:C     | 32:BF:23:ASP:H    | 2.01                     | 0.62              |
| 35:BI:140:LEU:HD12 | 35:BI:141:LYS:N   | 2.15                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BP:23:PRO:CD   | 38:BP:33:ARG:NE    | 2.58                     | 0.62              |
| 42:BT:41:ARG:C    | 42:BT:41:ARG:HD2   | 2.19                     | 0.62              |
| 47:BY:38:ILE:O    | 47:BY:39:VAL:HB    | 2.00                     | 0.62              |
| 1:CA:1350:A:H2'   | 1:CA:1351:U:O4'    | 1.99                     | 0.62              |
| 1:CA:507:C:H2'    | 1:CA:508:C:C5      | 2.30                     | 0.62              |
| 9:CI:82:ALA:C     | 9:CI:84:ALA:H      | 2.02                     | 0.62              |
| 10:CJ:34:VAL:CG2  | 10:CJ:74:ILE:HG22  | 2.28                     | 0.62              |
| 27:DA:2262:U:P    | 49:D0:19:LYS:NZ    | 2.73                     | 0.62              |
| 49:D0:20:ARG:NH1  | 49:D0:20:ARG:HG3   | 2.14                     | 0.62              |
| 50:D1:80:LEU:O    | 50:D1:82:LEU:HD22  | 2.00                     | 0.62              |
| 27:DA:1005:C:H1'  | 27:DA:1012:U:N3    | 2.14                     | 0.62              |
| 27:DA:113:G:H5''  | 27:DA:114:U:OP1    | 2.00                     | 0.62              |
| 27:DA:1183:G:O2'  | 27:DA:1184:G:H5'   | 2.00                     | 0.62              |
| 27:DA:1358:G:O2'  | 27:DA:1359:A:H5''  | 1.99                     | 0.62              |
| 27:DA:1484:G:H3'  | 27:DA:1485:G:C5'   | 2.29                     | 0.62              |
| 27:DA:2552:U:C2   | 27:DA:2554:U:H5''  | 2.34                     | 0.62              |
| 27:DA:2586:C:H2'  | 27:DA:2587:A:H5'   | 1.81                     | 0.62              |
| 27:DA:911:A:H2'   | 39:DQ:9:TYR:CE1    | 2.34                     | 0.62              |
| 29:DC:20:TYR:HE1  | 29:DC:22:ILE:HD13  | 1.65                     | 0.62              |
| 34:DH:102:ALA:HA  | 34:DH:117:PRO:HD3  | 1.80                     | 0.62              |
| 38:DP:82:GLY:HA2  | 38:DP:113:LYS:O    | 2.00                     | 0.62              |
| 44:DV:1:MET:HB2   | 44:DV:99:ILE:HG13  | 1.80                     | 0.62              |
| 1:AA:1190:G:OP1   | 3:AC:4:LYS:HA      | 2.00                     | 0.62              |
| 1:AA:1508:G:O2'   | 1:AA:1509:C:H5'    | 2.00                     | 0.62              |
| 1:AA:346:G:N3     | 1:AA:346:G:C2'     | 2.62                     | 0.62              |
| 4:AD:9:CYS:HB2    | 4:AD:22:LYS:HZ3    | 1.65                     | 0.62              |
| 5:AE:126:ARG:HG3  | 5:AE:126:ARG:HH11  | 1.64                     | 0.62              |
| 11:AK:22:HIS:HB3  | 11:AK:29:ILE:HG23  | 1.82                     | 0.62              |
| 13:AM:3:ARG:NH2   | 13:AM:7:VAL:HG13   | 2.15                     | 0.62              |
| 16:AP:82:GLN:NE2  | 16:AP:82:GLN:H     | 1.98                     | 0.62              |
| 49:B0:53:MET:HB2  | 49:B0:59:LEU:HD23  | 1.80                     | 0.62              |
| 58:B9:11:CYS:SG   | 58:B9:32:HIS:CE1   | 2.93                     | 0.62              |
| 27:BA:1557:C:H5'' | 27:BA:1558:A:OP2   | 2.00                     | 0.62              |
| 27:BA:1739:U:O2'  | 27:BA:1740:G:H5''  | 1.99                     | 0.62              |
| 27:BA:1887:C:C3'  | 27:BA:1888:G:H5''  | 2.30                     | 0.62              |
| 27:BA:250:G:H2'   | 27:BA:251:A:C8     | 2.33                     | 0.62              |
| 27:BA:92:A:H1'    | 27:BA:93:G:H8      | 1.65                     | 0.62              |
| 27:BA:1799:G:H2'  | 30:BD:181:GLU:OE2  | 2.00                     | 0.62              |
| 30:BD:261:LYS:HE2 | 30:BD:263:ARG:HH22 | 1.65                     | 0.62              |
| 31:BE:57:LYS:HA   | 31:BE:59:VAL:HG12  | 1.81                     | 0.62              |
| 32:BF:164:ARG:CG  | 32:BF:164:ARG:HH11 | 2.13                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:BF:63:LYS:HD3   | 32:BF:67:GLN:HB3   | 1.82                     | 0.62              |
| 33:BG:6:ALA:O      | 33:BG:9:ARG:HB2    | 2.00                     | 0.62              |
| 33:BG:75:LYS:HE3   | 33:BG:76:SER:H     | 1.63                     | 0.62              |
| 34:BH:154:PRO:O    | 34:BH:155:SER:O    | 2.18                     | 0.62              |
| 35:BI:91:SER:O     | 35:BI:92:VAL:CB    | 2.47                     | 0.62              |
| 36:BN:85:ILE:HG21  | 36:BN:90:MET:HE2   | 1.82                     | 0.62              |
| 38:BP:97:PRO:HD3   | 38:BP:126:VAL:O    | 1.99                     | 0.62              |
| 43:BU:92:ARG:NH2   | 44:BV:11:GLN:H     | 1.97                     | 0.62              |
| 1:CA:273:A:O2'     | 1:CA:274:A:H5'     | 2.00                     | 0.62              |
| 1:CA:557:G:C6      | 1:CA:558:G:C6      | 2.88                     | 0.62              |
| 1:CA:763:G:H2'     | 1:CA:764:C:H6      | 1.61                     | 0.62              |
| 3:CC:24:ALA:CB     | 3:CC:32:LEU:HD12   | 2.30                     | 0.62              |
| 3:CC:22:TRP:CD1    | 3:CC:57:ILE:O      | 2.53                     | 0.62              |
| 7:CG:108:ALA:O     | 7:CG:111:ARG:HG3   | 2.00                     | 0.62              |
| 1:CA:1298:C:H2'    | 7:CG:114:ARG:HH12  | 1.64                     | 0.62              |
| 9:CI:97:LYS:HB2    | 9:CI:97:LYS:NZ     | 2.13                     | 0.62              |
| 11:CK:126:ARG:C    | 11:CK:128:ALA:H    | 2.03                     | 0.62              |
| 13:CM:66:LEU:HD12  | 13:CM:66:LEU:N     | 2.15                     | 0.62              |
| 15:CO:7:GLU:O      | 15:CO:10:LYS:HG3   | 2.00                     | 0.62              |
| 56:D7:8:ASN:C      | 56:D7:8:ASN:HD22   | 2.02                     | 0.62              |
| 58:D9:24:TYR:O     | 58:D9:25:VAL:HG23  | 2.00                     | 0.62              |
| 27:DA:1655:A:H2    | 27:DA:2049:G:O3'   | 1.82                     | 0.62              |
| 27:DA:1816:G:O6    | 30:DD:37:LEU:HD11  | 2.00                     | 0.62              |
| 27:DA:195:A:N7     | 27:DA:197:A:OP1    | 2.33                     | 0.62              |
| 27:DA:2176:A:H2'   | 27:DA:2177:C:C6    | 2.35                     | 0.62              |
| 27:DA:2225:A:H4'   | 27:DA:2226:C:H6    | 1.65                     | 0.62              |
| 27:DA:577:G:O5'    | 27:DA:577:G:H8     | 1.83                     | 0.62              |
| 31:DE:1:MET:H2     | 31:DE:84:PHE:HB2   | 1.65                     | 0.62              |
| 32:DF:110:LEU:HD13 | 32:DF:110:LEU:O    | 1.99                     | 0.62              |
| 34:DH:98:LEU:HD12  | 34:DH:102:ALA:O    | 2.00                     | 0.62              |
| 36:DN:3:THR:O      | 36:DN:5:VAL:N      | 2.32                     | 0.62              |
| 39:DQ:16:ARG:CG    | 39:DQ:17:LEU:H     | 2.00                     | 0.62              |
| 43:DU:91:ASP:O     | 43:DU:92:ARG:HD3   | 2.00                     | 0.62              |
| 47:DY:46:LYS:H     | 47:DY:62:GLU:CD    | 2.03                     | 0.62              |
| 48:DZ:110:VAL:O    | 48:DZ:110:VAL:HG13 | 1.99                     | 0.62              |
| 1:AA:711:G:H2'     | 1:AA:712:A:C8      | 2.35                     | 0.61              |
| 7:AG:145:ALA:O     | 7:AG:146:GLU:HB2   | 2.00                     | 0.61              |
| 8:AH:132:GLU:HG2   | 8:AH:134:ILE:CD1   | 2.29                     | 0.61              |
| 15:AO:35:ARG:CZ    | 15:AO:35:ARG:HB3   | 2.30                     | 0.61              |
| 19:AS:40:ILE:HB    | 19:AS:67:VAL:O     | 2.00                     | 0.61              |
| 54:B5:34:PRO:O     | 54:B5:36:CYS:N     | 2.32                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:749:C:H4'   | 27:BA:1271:G:N3    | 2.15                     | 0.61              |
| 27:BA:1433:U:H5'' | 27:BA:1433:U:H6    | 1.64                     | 0.61              |
| 27:BA:2392:A:OP2  | 57:B8:31:HIS:HE1   | 1.82                     | 0.61              |
| 27:BA:924:C:H2'   | 27:BA:925:C:C6     | 2.35                     | 0.61              |
| 27:BA:2591:C:OP1  | 30:BD:239:ARG:HG2  | 1.99                     | 0.61              |
| 33:BG:91:ARG:HD2  | 33:BG:92:VAL:N     | 2.14                     | 0.61              |
| 34:BH:149:ARG:HA  | 34:BH:162:ILE:HD12 | 1.82                     | 0.61              |
| 34:BH:43:VAL:HB   | 34:BH:52:VAL:HA    | 1.81                     | 0.61              |
| 42:BT:16:ARG:H    | 42:BT:79:HIS:HD2   | 1.46                     | 0.61              |
| 43:BU:50:ARG:O    | 43:BU:54:LYS:NZ    | 2.29                     | 0.61              |
| 47:BY:28:LYS:O    | 47:BY:29:GLU:C     | 2.39                     | 0.61              |
| 1:CA:1315:U:O2'   | 1:CA:1316:G:H5'    | 2.00                     | 0.61              |
| 4:CD:101:LEU:HD23 | 4:CD:135:LEU:O     | 2.00                     | 0.61              |
| 4:CD:26:CYS:O     | 4:CD:31:CYS:HB2    | 2.00                     | 0.61              |
| 5:CE:103:GLY:O    | 5:CE:105:VAL:N     | 2.32                     | 0.61              |
| 7:CG:86:GLN:HE22  | 25:CY:30:A:H2      | 1.47                     | 0.61              |
| 8:CH:84:ARG:HG2   | 8:CH:86:ILE:HD11   | 1.82                     | 0.61              |
| 12:CL:82:ILE:HG23 | 12:CL:95:TYR:HB3   | 1.81                     | 0.61              |
| 13:CM:25:ILE:N    | 13:CM:25:ILE:HD12  | 2.15                     | 0.61              |
| 14:CN:26:ARG:HD3  | 14:CN:43:CYS:SG    | 2.40                     | 0.61              |
| 18:CR:62:GLU:HA   | 18:CR:65:ILE:CD1   | 2.30                     | 0.61              |
| 19:CS:20:LEU:CA   | 19:CS:23:ASN:HD22  | 2.12                     | 0.61              |
| 23:CW:56:G:H2'    | 23:CW:57:A:C5'     | 2.30                     | 0.61              |
| 25:CY:14:A:H3'    | 25:CY:15:G:C8      | 2.35                     | 0.61              |
| 25:CY:52:G:H2'    | 25:CY:53:U:H6      | 1.65                     | 0.61              |
| 52:D3:23:LEU:H    | 52:D3:23:LEU:CD1   | 2.12                     | 0.61              |
| 27:DA:108:U:H2'   | 27:DA:109:G:H8     | 1.65                     | 0.61              |
| 27:DA:1458:C:H4'  | 27:DA:1459:G:O5'   | 2.00                     | 0.61              |
| 27:DA:2121:G:H2'  | 27:DA:2122:U:C6    | 2.35                     | 0.61              |
| 27:DA:2252:G:O2'  | 27:DA:2253:G:H5'   | 2.00                     | 0.61              |
| 27:DA:2505:G:O6   | 27:DA:2576:G:H2'   | 2.00                     | 0.61              |
| 27:DA:2536:G:H2'  | 27:DA:2537:U:O4'   | 1.99                     | 0.61              |
| 27:DA:292:C:H2'   | 27:DA:292:C:O2     | 2.00                     | 0.61              |
| 27:DA:314:A:O2'   | 27:DA:315:G:H5'    | 1.99                     | 0.61              |
| 27:DA:631:A:C2'   | 27:DA:632:A:O5'    | 2.48                     | 0.61              |
| 28:DB:98:G:H2'    | 28:DB:99:G:C8      | 2.35                     | 0.61              |
| 30:DD:43:ARG:HH11 | 30:DD:44:ASN:HD21  | 1.40                     | 0.61              |
| 33:DG:39:ILE:HD11 | 33:DG:155:MET:SD   | 2.40                     | 0.61              |
| 33:DG:72:ARG:HD3  | 33:DG:86:MET:HA    | 1.82                     | 0.61              |
| 34:DH:68:THR:HG22 | 34:DH:72:ILE:HD11  | 1.82                     | 0.61              |
| 37:DO:101:PRO:C   | 37:DO:102:VAL:HG12 | 2.19                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DR:54:LEU:HD23 | 40:DR:66:VAL:HG22  | 1.81                     | 0.61              |
| 40:DR:94:TYR:HD1  | 40:DR:94:TYR:H     | 1.47                     | 0.61              |
| 42:DT:74:ARG:HD3  | 42:DT:76:PHE:CE2   | 2.34                     | 0.61              |
| 42:DT:7:ILE:O     | 42:DT:11:GLU:OE2   | 2.18                     | 0.61              |
| 44:DV:1:MET:HA    | 44:DV:1:MET:CE     | 2.29                     | 0.61              |
| 1:AA:1206:G:C2'   | 1:AA:1207:G:H5'    | 2.31                     | 0.61              |
| 1:AA:1298:C:C4    | 7:AG:114:ARG:HD2   | 2.36                     | 0.61              |
| 1:AA:160:A:H1'    | 1:AA:344:A:C4      | 2.35                     | 0.61              |
| 5:AE:76:ILE:HD11  | 5:AE:142:LEU:HD22  | 1.82                     | 0.61              |
| 17:AQ:68:ARG:N    | 17:AQ:70:ARG:NH1   | 2.48                     | 0.61              |
| 58:B9:11:CYS:SG   | 58:B9:32:HIS:ND1   | 2.73                     | 0.61              |
| 27:BA:2308:G:H2'  | 27:BA:2309:A:O5'   | 2.00                     | 0.61              |
| 27:BA:2855:C:O2'  | 27:BA:2856:C:H5'   | 2.00                     | 0.61              |
| 27:BA:27:G:O2'    | 27:BA:28:A:C8      | 2.53                     | 0.61              |
| 27:BA:709:U:C4    | 27:BA:710:G:N7     | 2.68                     | 0.61              |
| 27:BA:854:G:H2'   | 27:BA:855:G:H8     | 1.65                     | 0.61              |
| 30:BD:46:GLN:OE1  | 30:BD:46:GLN:N     | 2.33                     | 0.61              |
| 32:BF:160:ASN:C   | 32:BF:162:LEU:H    | 2.02                     | 0.61              |
| 33:BG:103:LEU:H   | 33:BG:103:LEU:HD12 | 1.66                     | 0.61              |
| 33:BG:141:PHE:HB3 | 33:BG:142:PRO:HD2  | 1.82                     | 0.61              |
| 34:BH:119:GLU:HG2 | 34:BH:119:GLU:O    | 2.00                     | 0.61              |
| 35:BI:101:LEU:HG  | 35:BI:107:VAL:HB   | 1.82                     | 0.61              |
| 38:BP:64:LYS:O    | 38:BP:66:GLY:N     | 2.34                     | 0.61              |
| 40:BR:4:LEU:C     | 40:BR:6:SER:H      | 2.03                     | 0.61              |
| 1:CA:119:A:H5''   | 1:CA:120:A:H5'     | 1.82                     | 0.61              |
| 1:CA:1279:A:O2'   | 1:CA:1282:C:N4     | 2.32                     | 0.61              |
| 1:CA:1283:G:O2'   | 1:CA:1284:C:H5'    | 2.00                     | 0.61              |
| 1:CA:638:G:H2'    | 1:CA:639:G:H8      | 1.64                     | 0.61              |
| 1:CA:954:G:H2'    | 1:CA:955:U:C6      | 2.35                     | 0.61              |
| 15:CO:39:LEU:CD1  | 15:CO:56:LEU:HB2   | 2.29                     | 0.61              |
| 21:CU:6:ARG:HD3   | 21:CU:15:ARG:NH1   | 2.14                     | 0.61              |
| 27:DA:1292:U:H2'  | 27:DA:1293:C:C6    | 2.35                     | 0.61              |
| 27:DA:1473:G:O2'  | 27:DA:1474:C:H5'   | 2.00                     | 0.61              |
| 27:DA:1566:A:O2'  | 27:DA:1567:A:H5'   | 2.00                     | 0.61              |
| 27:DA:2027:G:H2'  | 27:DA:2028:U:O4'   | 2.00                     | 0.61              |
| 27:DA:315:G:H2'   | 27:DA:316:C:C6     | 2.34                     | 0.61              |
| 27:DA:64:A:O2'    | 27:DA:65:C:H5'     | 2.00                     | 0.61              |
| 27:DA:999:U:O2    | 27:DA:999:U:H2'    | 2.00                     | 0.61              |
| 29:DC:68:LEU:HD11 | 29:DC:179:SER:HA   | 1.81                     | 0.61              |
| 30:DD:69:ARG:NH2  | 30:DD:192:THR:HG21 | 2.14                     | 0.61              |
| 31:DE:79:ARG:HH12 | 31:DE:195:LEU:HD23 | 1.64                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DF:170:LEU:HB3  | 32:DF:173:VAL:HB  | 1.82                     | 0.61              |
| 33:DG:29:TRP:HA    | 33:DG:29:TRP:CE3  | 2.35                     | 0.61              |
| 34:DH:107:VAL:HG21 | 34:DH:152:ARG:CG  | 2.29                     | 0.61              |
| 34:DH:103:LEU:CD2  | 34:DH:115:VAL:HB  | 2.30                     | 0.61              |
| 40:DR:24:GLN:NE2   | 40:DR:36:THR:HG21 | 2.14                     | 0.61              |
| 41:DS:14:VAL:HG22  | 41:DS:91:PRO:HD3  | 1.82                     | 0.61              |
| 42:DT:83:ILE:HG13  | 42:DT:84:GLN:N    | 2.15                     | 0.61              |
| 48:DZ:18:ARG:HB3   | 48:DZ:81:ARG:NH2  | 2.13                     | 0.61              |
| 1:AA:243:A:H4'     | 1:AA:244:U:O5'    | 2.00                     | 0.61              |
| 1:AA:318:G:O2'     | 1:AA:319:G:H5'    | 2.00                     | 0.61              |
| 10:AJ:22:LYS:O     | 10:AJ:22:LYS:HD2  | 1.99                     | 0.61              |
| 14:AN:57:ARG:O     | 14:AN:59:ALA:N    | 2.33                     | 0.61              |
| 19:AS:62:ILE:HG23  | 19:AS:62:ILE:O    | 1.99                     | 0.61              |
| 19:AS:6:LYS:HG2    | 19:AS:7:LYS:HE2   | 1.81                     | 0.61              |
| 50:B1:84:GLY:O     | 50:B1:86:SER:N    | 2.33                     | 0.61              |
| 53:B4:46:ASN:ND2   | 53:B4:47:VAL:N    | 2.48                     | 0.61              |
| 27:BA:1021:A:H3'   | 27:BA:1021:A:H8   | 1.64                     | 0.61              |
| 27:BA:1309:G:O2'   | 27:BA:1310:G:H5'  | 1.99                     | 0.61              |
| 27:BA:1336:A:O2'   | 27:BA:1337:G:H5'  | 2.00                     | 0.61              |
| 27:BA:1677:A:H2'   | 27:BA:1678:G:H8   | 1.64                     | 0.61              |
| 27:BA:2131:G:H5'   | 27:BA:2133:G:O5'  | 2.00                     | 0.61              |
| 27:BA:2338:G:O2'   | 27:BA:2339:G:H5'  | 2.01                     | 0.61              |
| 27:BA:1709:U:H1'   | 27:BA:2860:A:H1'  | 1.82                     | 0.61              |
| 27:BA:42:G:H2'     | 27:BA:43:A:O4'    | 2.00                     | 0.61              |
| 27:BA:732:C:H2'    | 27:BA:733:G:O4'   | 1.99                     | 0.61              |
| 27:BA:787:U:H5''   | 27:BA:788:A:H5'   | 1.81                     | 0.61              |
| 30:BD:31:LYS:HG3   | 30:BD:33:LEU:HB2  | 1.82                     | 0.61              |
| 31:BE:173:VAL:O    | 31:BE:174:ASP:O   | 2.18                     | 0.61              |
| 32:BF:200:GLU:HA   | 32:BF:203:GLN:HB2 | 1.82                     | 0.61              |
| 38:BP:23:PRO:CD    | 38:BP:33:ARG:CZ   | 2.78                     | 0.61              |
| 38:BP:97:PRO:C     | 38:BP:98:GLU:CG   | 2.68                     | 0.61              |
| 39:BQ:78:PRO:HD2   | 39:BQ:81:VAL:HG11 | 1.82                     | 0.61              |
| 42:BT:28:VAL:HG13  | 42:BT:46:GLU:HA   | 1.83                     | 0.61              |
| 44:BV:28:GLU:HB3   | 44:BV:29:PRO:HD2  | 1.82                     | 0.61              |
| 48:BZ:116:LEU:HD21 | 48:BZ:171:ALA:HB1 | 1.83                     | 0.61              |
| 1:CA:1106:G:H5''   | 3:CC:172:ARG:CG   | 2.23                     | 0.61              |
| 1:CA:946:A:O2'     | 1:CA:1333:A:N3    | 2.30                     | 0.61              |
| 1:CA:243:A:O2'     | 1:CA:244:U:OP2    | 2.17                     | 0.61              |
| 1:CA:27:G:H4'      | 4:CD:209:ARG:OXT  | 2.00                     | 0.61              |
| 1:CA:34:C:O2'      | 1:CA:35:G:H5'     | 2.00                     | 0.61              |
| 1:CA:407:G:O2'     | 1:CA:408:A:H5'    | 2.00                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CB:16:HIS:HB3    | 2:CB:210:SER:HB3   | 1.82                     | 0.61              |
| 3:CC:181:ASN:OD1   | 3:CC:204:LEU:HD12  | 2.00                     | 0.61              |
| 5:CE:76:ILE:HD11   | 5:CE:142:LEU:CD1   | 2.30                     | 0.61              |
| 1:CA:1251:A:H5''   | 9:CI:12:GLU:OE1    | 2.01                     | 0.61              |
| 1:CA:134:A:N6      | 16:CP:25:ARG:HH12  | 1.98                     | 0.61              |
| 23:CW:10:G:N1      | 23:CW:25:A:H1'     | 2.16                     | 0.61              |
| 57:D8:52:LYS:N     | 57:D8:53:PRO:CD    | 2.59                     | 0.61              |
| 27:DA:1191:G:O2'   | 27:DA:1192:G:H5'   | 1.99                     | 0.61              |
| 27:DA:1685:C:H2'   | 27:DA:1686:C:H5''  | 1.82                     | 0.61              |
| 27:DA:2161:C:H2'   | 27:DA:2162:G:H8    | 1.59                     | 0.61              |
| 27:DA:2360:A:H8    | 27:DA:2360:A:O5'   | 1.83                     | 0.61              |
| 27:DA:2550:G:N2    | 27:DA:2559:C:H1'   | 2.12                     | 0.61              |
| 30:DD:26:LYS:HG2   | 30:DD:26:LYS:O     | 2.00                     | 0.61              |
| 30:DD:32:SER:O     | 30:DD:34:VAL:N     | 2.33                     | 0.61              |
| 30:DD:65:ILE:HG22  | 30:DD:104:TYR:HB3  | 1.82                     | 0.61              |
| 30:DD:69:ARG:HH22  | 30:DD:192:THR:HG21 | 1.65                     | 0.61              |
| 13:CM:7:VAL:HG21   | 33:DG:115:ARG:HG2  | 1.82                     | 0.61              |
| 38:DP:146:VAL:HG13 | 38:DP:147:LEU:H    | 1.65                     | 0.61              |
| 40:DR:38:VAL:CB    | 40:DR:39:PRO:HD3   | 2.23                     | 0.61              |
| 44:DV:71:LEU:CD1   | 44:DV:84:LYS:HE2   | 2.31                     | 0.61              |
| 1:AA:1313:U:P      | 19:AS:6:LYS:HG3    | 2.40                     | 0.61              |
| 1:AA:189(F):U:O2'  | 17:AQ:63:ARG:NH2   | 2.34                     | 0.61              |
| 1:AA:818:G:O2'     | 1:AA:819:A:H5''    | 1.98                     | 0.61              |
| 2:AB:98:LEU:O      | 2:AB:101:MET:HG3   | 2.01                     | 0.61              |
| 3:AC:5:ILE:HD12    | 3:AC:5:ILE:O       | 2.00                     | 0.61              |
| 4:AD:153:ARG:NH2   | 4:AD:181:MET:HB2   | 2.15                     | 0.61              |
| 4:AD:86:LYS:HD3    | 4:AD:87:GLY:H      | 1.65                     | 0.61              |
| 6:AF:69:GLU:CD     | 6:AF:69:GLU:H      | 2.03                     | 0.61              |
| 12:AL:43:LYS:HG2   | 12:AL:44:LYS:H     | 1.64                     | 0.61              |
| 17:AQ:26:GLN:HE21  | 17:AQ:37:LYS:HG2   | 1.65                     | 0.61              |
| 17:AQ:59:ILE:CG2   | 17:AQ:71:PHE:HB3   | 2.30                     | 0.61              |
| 17:AQ:56:VAL:CG2   | 17:AQ:78:GLU:HG2   | 2.31                     | 0.61              |
| 49:B0:71:ASP:O     | 49:B0:73:GLY:N     | 2.34                     | 0.61              |
| 57:B8:28:GLY:C     | 57:B8:32:LEU:HD23  | 2.20                     | 0.61              |
| 57:B8:50:LEU:HA    | 57:B8:53:PRO:HG3   | 1.81                     | 0.61              |
| 27:BA:1286:A:O2'   | 27:BA:1288:U:OP2   | 2.17                     | 0.61              |
| 27:BA:1503:U:H2'   | 27:BA:1504:C:C6    | 2.34                     | 0.61              |
| 27:BA:181:A:C2     | 27:BA:182:A:C4     | 2.89                     | 0.61              |
| 27:BA:2479:G:OP1   | 27:BA:2537:U:H1'   | 2.00                     | 0.61              |
| 27:BA:854:G:H2'    | 27:BA:855:G:C8     | 2.34                     | 0.61              |
| 30:BD:26:LYS:HZ3   | 30:BD:81:ALA:HB1   | 1.64                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BH:154:PRO:HB3 | 34:BH:163:TYR:CZ  | 2.35                     | 0.61              |
| 34:BH:43:VAL:HG11 | 34:BH:52:VAL:CG1  | 2.29                     | 0.61              |
| 1:CA:1402:C:H2'   | 1:CA:1403:C:O4'   | 2.00                     | 0.61              |
| 1:CA:1478:C:H2'   | 1:CA:1479:C:H6    | 1.65                     | 0.61              |
| 1:CA:578:C:H2'    | 1:CA:578:C:O2     | 2.00                     | 0.61              |
| 1:CA:750:G:N2     | 15:CO:23:GLY:HA3  | 2.15                     | 0.61              |
| 1:CA:777:A:O2'    | 1:CA:778:G:H5'    | 2.00                     | 0.61              |
| 4:CD:173:TRP:HA   | 4:CD:187:ARG:HH12 | 1.64                     | 0.61              |
| 5:CE:88:LYS:HB3   | 5:CE:123:LEU:HB2  | 1.81                     | 0.61              |
| 8:CH:12:ARG:HA    | 8:CH:15:ASN:HD22  | 1.65                     | 0.61              |
| 12:CL:76:GLU:O    | 12:CL:77:HIS:CB   | 2.46                     | 0.61              |
| 14:CN:37:PHE:CB   | 14:CN:39:LEU:HG   | 2.21                     | 0.61              |
| 14:CN:57:ARG:HG2  | 14:CN:58:LYS:N    | 2.15                     | 0.61              |
| 15:CO:35:ARG:O    | 15:CO:39:LEU:HB2  | 2.00                     | 0.61              |
| 15:CO:36:ILE:HG22 | 15:CO:37:ASN:N    | 2.14                     | 0.61              |
| 1:CA:564:C:C5     | 17:CQ:31:LEU:HD11 | 2.36                     | 0.61              |
| 17:CQ:77:VAL:O    | 17:CQ:78:GLU:HB3  | 2.00                     | 0.61              |
| 23:CW:67:C:H2'    | 23:CW:68:C:C6     | 2.35                     | 0.61              |
| 54:D5:25:LEU:CD2  | 54:D5:26:THR:H    | 2.14                     | 0.61              |
| 57:D8:37:SER:O    | 57:D8:40:GLU:HB2  | 2.01                     | 0.61              |
| 27:DA:1011:G:OP1  | 43:DU:77:SER:N    | 2.26                     | 0.61              |
| 27:DA:2067:G:H1   | 27:DA:2443:C:H42  | 1.48                     | 0.61              |
| 27:DA:2454:G:H2'  | 27:DA:2455:G:O4'  | 2.00                     | 0.61              |
| 27:DA:2733:A:H2   | 31:DE:203:LYS:HA  | 1.64                     | 0.61              |
| 27:DA:319:C:H2'   | 27:DA:320:A:H8    | 1.64                     | 0.61              |
| 27:DA:915:C:N4    | 27:DA:916:G:C6    | 2.68                     | 0.61              |
| 32:DF:32:LEU:O    | 32:DF:36:VAL:HG23 | 1.99                     | 0.61              |
| 37:DO:16:ALA:HA   | 37:DO:46:ALA:CB   | 2.31                     | 0.61              |
| 38:DP:115:LEU:HG  | 38:DP:116:GLY:N   | 2.15                     | 0.61              |
| 38:DP:126:VAL:HA  | 38:DP:145:PRO:HB2 | 1.81                     | 0.61              |
| 40:DR:6:SER:O     | 40:DR:7:GLY:O     | 2.18                     | 0.61              |
| 44:DV:3:ALA:HB2   | 44:DV:99:ILE:HG21 | 1.83                     | 0.61              |
| 27:DA:139(A):G:N2 | 46:DX:44:GLU:OE1  | 2.32                     | 0.61              |
| 47:DY:46:LYS:HD3  | 47:DY:47:LYS:NZ   | 2.15                     | 0.61              |
| 1:AA:1319:A:H4'   | 1:AA:1320:C:OP1   | 2.01                     | 0.61              |
| 1:AA:116:A:H61    | 1:AA:313:A:H1'    | 1.66                     | 0.61              |
| 1:AA:531:U:H4'    | 1:AA:532:A:O5'    | 2.01                     | 0.61              |
| 5:AE:92:LYS:O     | 5:AE:118:ILE:HD12 | 1.99                     | 0.61              |
| 9:AI:91:ASP:C     | 9:AI:93:ARG:H     | 2.04                     | 0.61              |
| 52:B3:23:LEU:HB3  | 52:B3:28:LEU:HB2  | 1.82                     | 0.61              |
| 27:BA:1345:C:H2'  | 27:BA:1346:G:C8   | 2.34                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:1755:A:H2'   | 27:BA:1756:G:H5'  | 1.83                     | 0.61              |
| 27:BA:2197:U:H1'   | 27:BA:2198:A:C8   | 2.36                     | 0.61              |
| 27:BA:576:U:O2'    | 27:BA:577:G:H5'   | 2.01                     | 0.61              |
| 27:BA:97:C:H5''    | 51:B2:2:LYS:HB2   | 1.83                     | 0.61              |
| 31:BE:132:HIS:CD2  | 31:BE:135:HIS:CE1 | 2.88                     | 0.61              |
| 37:BO:2:ILE:O      | 37:BO:32:TYR:HB3  | 1.99                     | 0.61              |
| 41:BS:17:ARG:O     | 41:BS:18:ILE:CB   | 2.48                     | 0.61              |
| 42:BT:92:GLY:O     | 42:BT:94:ALA:N    | 2.34                     | 0.61              |
| 45:BW:90:ARG:HG3   | 45:BW:90:ARG:HH11 | 1.65                     | 0.61              |
| 47:BY:87:LYS:HG3   | 47:BY:88:LYS:N    | 2.15                     | 0.61              |
| 1:CA:59:A:H1'      | 1:CA:354:G:N2     | 2.15                     | 0.61              |
| 1:CA:726:C:O2'     | 1:CA:727:G:H5'    | 2.00                     | 0.61              |
| 2:CB:92:TYR:C      | 2:CB:92:TYR:CD1   | 2.73                     | 0.61              |
| 2:CB:92:TYR:C      | 2:CB:92:TYR:HD1   | 2.03                     | 0.61              |
| 9:CI:9:ARG:HG3     | 9:CI:14:VAL:CG2   | 2.29                     | 0.61              |
| 12:CL:3:THR:HG23   | 12:CL:6:GLN:HB2   | 1.82                     | 0.61              |
| 18:CR:82:THR:C     | 18:CR:83:GLU:HG2  | 2.20                     | 0.61              |
| 23:CW:28:G:H3'     | 23:CW:29:G:H8     | 1.64                     | 0.61              |
| 23:CW:34:U:O2'     | 23:CW:35:G:H5'    | 2.00                     | 0.61              |
| 23:CW:57:A:H3'     | 23:CW:57:A:OP1    | 2.00                     | 0.61              |
| 27:DA:1033:U:O4    | 58:D9:15:LYS:HE3  | 1.99                     | 0.61              |
| 27:DA:125:G:H1'    | 56:D7:13:ALA:HB1  | 1.82                     | 0.61              |
| 27:DA:2405:G:HO2'  | 27:DA:2406:U:P    | 2.24                     | 0.61              |
| 27:DA:2531:A:H61   | 27:DA:2662:A:H61  | 1.48                     | 0.61              |
| 27:DA:272(C):G:H1  | 27:DA:365:C:N4    | 1.95                     | 0.61              |
| 27:DA:50:U:C4'     | 27:DA:51:G:OP2    | 2.47                     | 0.61              |
| 31:DE:93:VAL:O     | 31:DE:95:ILE:N    | 2.33                     | 0.61              |
| 34:DH:89:ILE:HG12  | 34:DH:129:THR:HA  | 1.82                     | 0.61              |
| 36:DN:19:GLU:HG3   | 36:DN:20:GLY:N    | 2.15                     | 0.61              |
| 38:DP:135:LEU:HD13 | 38:DP:135:LEU:O   | 1.99                     | 0.61              |
| 41:DS:62:LYS:H     | 41:DS:65:VAL:HG23 | 1.65                     | 0.61              |
| 46:DX:57:LEU:HD22  | 46:DX:57:LEU:C    | 2.21                     | 0.61              |
| 48:DZ:107:PRO:HG3  | 48:DZ:116:LEU:HB2 | 1.82                     | 0.61              |
| 48:DZ:7:TYR:CD1    | 48:DZ:7:TYR:N     | 2.68                     | 0.61              |
| 1:AA:920:U:O4'     | 1:AA:1080:A:C2    | 2.54                     | 0.61              |
| 1:AA:1233:G:H2'    | 1:AA:1234:C:C6    | 2.34                     | 0.61              |
| 1:AA:889:A:H4'     | 1:AA:890:G:OP1    | 2.01                     | 0.61              |
| 6:AF:43:LEU:CD1    | 6:AF:43:LEU:H     | 2.01                     | 0.61              |
| 10:AJ:90:LEU:N     | 10:AJ:91:PRO:CD   | 2.64                     | 0.61              |
| 16:AP:20:VAL:HG21  | 16:AP:32:TYR:CD1  | 2.36                     | 0.61              |
| 17:AQ:3:LYS:HD2    | 17:AQ:60:ILE:HD11 | 1.82                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AY:35:G:H2'     | 25:AY:36:A:C8      | 2.36                     | 0.61              |
| 50:B1:75:GLU:O     | 50:B1:77:ALA:N     | 2.32                     | 0.61              |
| 27:BA:466:A:H2'    | 27:BA:467:G:H5'    | 1.83                     | 0.61              |
| 27:BA:910:A:H62    | 39:BQ:12:GLN:HA    | 1.64                     | 0.61              |
| 27:BA:942:G:O2'    | 27:BA:943:U:H5'    | 2.00                     | 0.61              |
| 32:BF:186:ILE:HD13 | 32:BF:192:LEU:CD1  | 2.31                     | 0.61              |
| 28:BB:42:C:H4'     | 33:BG:67:LYS:O     | 2.01                     | 0.61              |
| 36:BN:29:LYS:O     | 36:BN:33:LEU:HD12  | 2.00                     | 0.61              |
| 36:BN:57:ALA:H     | 36:BN:124:ALA:HA   | 1.65                     | 0.61              |
| 37:BO:75:SER:O     | 37:BO:76:ALA:HB2   | 2.01                     | 0.61              |
| 27:BA:2415:G:O3'   | 38:BP:66:GLY:HA3   | 1.99                     | 0.61              |
| 48:BZ:140:VAL:O    | 48:BZ:140:VAL:HG22 | 2.01                     | 0.61              |
| 1:CA:15:G:H1       | 1:CA:920:U:H3      | 1.47                     | 0.61              |
| 1:CA:60:A:C5'      | 1:CA:331:G:H22     | 2.13                     | 0.61              |
| 1:CA:503:C:O2'     | 1:CA:504:C:H5'     | 2.01                     | 0.61              |
| 10:CJ:78:ASN:HD22  | 10:CJ:80:LYS:H     | 1.49                     | 0.61              |
| 12:CL:45:PRO:CB    | 22:CV:9:G:H4'      | 2.29                     | 0.61              |
| 13:CM:68:GLY:C     | 13:CM:71:ARG:HB3   | 2.20                     | 0.61              |
| 14:CN:24:CYS:CB    | 14:CN:40:CYS:HB3   | 2.31                     | 0.61              |
| 18:CR:35:ARG:O     | 18:CR:37:VAL:HG13  | 2.00                     | 0.61              |
| 27:DA:849:A:N1     | 52:D3:25:ALA:HB2   | 2.14                     | 0.61              |
| 58:D9:18:ARG:O     | 58:D9:18:ARG:CG    | 2.47                     | 0.61              |
| 27:DA:1176:G:O2'   | 27:DA:1177:A:H5'   | 2.00                     | 0.61              |
| 27:DA:1424:G:H2'   | 27:DA:1425:G:O4'   | 1.99                     | 0.61              |
| 27:DA:1657:C:H2'   | 27:DA:1658:C:C6    | 2.36                     | 0.61              |
| 27:DA:1933:G:H2'   | 27:DA:1934:C:C6    | 2.35                     | 0.61              |
| 27:DA:2160:G:H2'   | 27:DA:2161:C:C6    | 2.36                     | 0.61              |
| 27:DA:2192:G:C2'   | 27:DA:2193:G:H5''  | 2.30                     | 0.61              |
| 27:DA:2691:C:H42   | 27:DA:2718:G:H1    | 1.49                     | 0.61              |
| 27:DA:376:C:H2'    | 27:DA:377:C:C6     | 2.35                     | 0.61              |
| 27:DA:27:G:H2'     | 27:DA:512:G:H22    | 1.63                     | 0.61              |
| 33:DG:36:LYS:HG2   | 33:DG:160:VAL:CG2  | 2.29                     | 0.61              |
| 38:DP:108:LYS:HD2  | 38:DP:108:LYS:H    | 1.64                     | 0.61              |
| 39:DQ:42:ILE:N     | 39:DQ:42:ILE:HD12  | 2.14                     | 0.61              |
| 42:DT:34:VAL:O     | 42:DT:34:VAL:HG12  | 1.99                     | 0.61              |
| 43:DU:92:ARG:NH1   | 44:DV:11:GLN:HG3   | 2.16                     | 0.61              |
| 44:DV:47:VAL:O     | 44:DV:48:GLY:C     | 2.38                     | 0.61              |
| 1:AA:1154:G:H2'    | 1:AA:1155:G:H8     | 1.64                     | 0.61              |
| 1:AA:1179:A:H5'    | 9:AI:102:LEU:HD12  | 1.83                     | 0.61              |
| 3:AC:19:GLU:O      | 3:AC:40:ARG:NH2    | 2.34                     | 0.61              |
| 7:AG:115:ARG:HB2   | 7:AG:118:VAL:HG13  | 1.82                     | 0.61              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:AJ:53:PRO:HA    | 14:AN:41:ARG:NH2    | 2.16                     | 0.61              |
| 11:AK:50:TYR:CB    | 11:AK:54:ARG:O      | 2.48                     | 0.61              |
| 25:AY:42:G:N2      | 25:AY:43:C:H1'      | 2.15                     | 0.61              |
| 56:B7:37:LYS:HD3   | 56:B7:39:ARG:HE     | 1.63                     | 0.61              |
| 58:B9:7:VAL:HG13   | 58:B9:34:GLN:NE2    | 2.14                     | 0.61              |
| 27:BA:1502:C:H2'   | 27:BA:1502:C:O2     | 2.00                     | 0.61              |
| 27:BA:1670:C:H42   | 27:BA:1674:G:H5'    | 1.65                     | 0.61              |
| 27:BA:1790:C:H5''  | 27:BA:1791:A:OP1    | 2.01                     | 0.61              |
| 27:BA:2619:C:H4'   | 31:BE:151:TYR:O     | 2.01                     | 0.61              |
| 27:BA:663:G:H2'    | 27:BA:664:C:H6      | 1.65                     | 0.61              |
| 27:BA:825:C:H2'    | 27:BA:826:U:O4'     | 1.99                     | 0.61              |
| 29:BC:45:ALA:O     | 29:BC:46:LYS:HB2    | 2.00                     | 0.61              |
| 30:BD:49:ILE:HD11  | 30:BD:52:ARG:CA     | 2.24                     | 0.61              |
| 31:BE:101:ARG:HH21 | 31:BE:171:GLU:HB2   | 1.66                     | 0.61              |
| 31:BE:68:ALA:C     | 31:BE:70:ALA:N      | 2.53                     | 0.61              |
| 32:BF:160:ASN:O    | 32:BF:162:LEU:N     | 2.34                     | 0.61              |
| 32:BF:40:GLN:HE22  | 32:BF:184:TYR:HB3   | 1.66                     | 0.61              |
| 33:BG:170:ARG:HH22 | 33:BG:182:LYS:HG3   | 1.64                     | 0.61              |
| 33:BG:52:ILE:HG22  | 33:BG:54:GLU:HG2    | 1.81                     | 0.61              |
| 36:BN:119:ARG:O    | 36:BN:120:LEU:CB    | 2.49                     | 0.61              |
| 27:BA:661:C:O2'    | 38:BP:16:ARG:O      | 2.12                     | 0.61              |
| 40:BR:98:LEU:CD1   | 40:BR:113:LEU:HD23  | 2.28                     | 0.61              |
| 43:BU:12:ARG:O     | 43:BU:15:LYS:HD3    | 2.01                     | 0.61              |
| 1:CA:225:C:H2'     | 1:CA:225:C:O2       | 2.01                     | 0.61              |
| 2:CB:82:ARG:HG3    | 2:CB:92:TYR:CE2     | 2.36                     | 0.61              |
| 6:CF:25:ILE:HD13   | 6:CF:28:ARG:HD2     | 1.82                     | 0.61              |
| 9:CI:15:ALA:HB2    | 9:CI:65:VAL:HG23    | 1.83                     | 0.61              |
| 6:CF:96:PRO:HB3    | 18:CR:30:ASP:OD2    | 1.99                     | 0.61              |
| 18:CR:35:ARG:O     | 18:CR:37:VAL:N      | 2.34                     | 0.61              |
| 23:CW:56:G:H2'     | 23:CW:57:A:H5'      | 1.81                     | 0.61              |
| 55:D6:13:CYS:HB3   | 55:D6:50:ARG:O      | 2.00                     | 0.61              |
| 56:D7:8:ASN:ND2    | 56:D7:11:LYS:N      | 2.44                     | 0.61              |
| 27:DA:243:U:OP1    | 57:D8:6:THR:HG21    | 2.00                     | 0.61              |
| 27:DA:1518:U:H2'   | 27:DA:1519:G:O4'    | 2.01                     | 0.61              |
| 27:DA:1702:G:H2'   | 27:DA:1703:G:O5'    | 2.00                     | 0.61              |
| 27:DA:2178:C:H5''  | 29:DC:46:LYS:HG2    | 1.81                     | 0.61              |
| 27:DA:2279:G:N2    | 27:DA:2280:G:H1'    | 2.15                     | 0.61              |
| 27:DA:244:A:C2     | 27:DA:255:A:C4      | 2.88                     | 0.61              |
| 27:DA:2668:G:O2'   | 27:DA:2669:G:H5'    | 2.00                     | 0.61              |
| 27:DA:2712:U:C2'   | 27:DA:2712(A):A:O5' | 2.48                     | 0.61              |
| 27:DA:777:A:O2'    | 27:DA:778:G:H5'     | 2.01                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:DB:26:A:C3'     | 28:DB:27:C:H5''   | 2.31                     | 0.61              |
| 33:DG:180:PHE:C    | 33:DG:182:LYS:H   | 2.04                     | 0.61              |
| 33:DG:71:THR:OG1   | 33:DG:89:GLY:HA3  | 2.01                     | 0.61              |
| 39:DQ:38:GLU:HG3   | 39:DQ:127:ILE:CB  | 2.31                     | 0.61              |
| 43:DU:42:ALA:C     | 43:DU:44:ASN:N    | 2.51                     | 0.61              |
| 45:DW:46:PHE:O     | 45:DW:50:VAL:HG12 | 2.01                     | 0.61              |
| 48:DZ:13:LYS:O     | 48:DZ:17:LEU:N    | 2.33                     | 0.61              |
| 1:AA:1139:G:H5'    | 1:AA:1140:C:OP1   | 2.01                     | 0.61              |
| 1:AA:376:G:H4'     | 16:AP:5:ARG:HD2   | 1.83                     | 0.61              |
| 1:AA:444:C:H42     | 1:AA:490:G:H1     | 1.48                     | 0.61              |
| 1:AA:511:C:HO2'    | 1:AA:512:U:H6     | 1.48                     | 0.61              |
| 1:AA:677:U:H3      | 1:AA:714:G:H22    | 1.48                     | 0.61              |
| 1:AA:952:U:O2'     | 1:AA:953:G:H5'    | 2.01                     | 0.61              |
| 13:AM:70:LEU:O     | 13:AM:74:VAL:HG23 | 1.99                     | 0.61              |
| 13:AM:23:TYR:HE1   | 13:AM:71:ARG:HB2  | 1.66                     | 0.61              |
| 16:AP:50:LYS:HD3   | 16:AP:50:LYS:C    | 2.20                     | 0.61              |
| 16:AP:6:LEU:H      | 16:AP:6:LEU:HD12  | 1.65                     | 0.61              |
| 50:B1:64:ALA:HA    | 50:B1:67:ILE:HG13 | 1.81                     | 0.61              |
| 27:BA:2815:C:H5'   | 54:B5:29:THR:HG21 | 1.82                     | 0.61              |
| 27:BA:1311:G:C6    | 56:B7:47:ARG:NH1  | 2.69                     | 0.61              |
| 27:BA:1050:A:HO2'  | 27:BA:1051:G:H8   | 1.43                     | 0.61              |
| 27:BA:996:A:N6     | 27:BA:1160:G:C6   | 2.68                     | 0.61              |
| 27:BA:125:G:N2     | 56:B7:48:LYS:NZ   | 2.49                     | 0.61              |
| 27:BA:1503:U:H2'   | 27:BA:1504:C:H6   | 1.66                     | 0.61              |
| 27:BA:1603:A:C5'   | 27:BA:1603:A:H8   | 2.14                     | 0.61              |
| 27:BA:1782:C:H1'   | 27:BA:2609:U:C5'  | 2.28                     | 0.61              |
| 27:BA:2432:A:H2'   | 27:BA:2433:A:H8   | 1.62                     | 0.61              |
| 27:BA:2828:C:O2'   | 27:BA:2829:C:H5'  | 2.01                     | 0.61              |
| 27:BA:548:A:O2'    | 27:BA:549:G:OP1   | 2.18                     | 0.61              |
| 29:BC:196:LEU:C    | 29:BC:198:ALA:N   | 2.49                     | 0.61              |
| 27:BA:2203:U:H4'   | 30:BD:151:LYS:HG2 | 1.82                     | 0.61              |
| 31:BE:130:GLY:O    | 31:BE:131:ALA:O   | 2.19                     | 0.61              |
| 32:BF:176:LEU:HD21 | 32:BF:180:GLY:O   | 2.01                     | 0.61              |
| 35:BI:114:LEU:O    | 35:BI:115:ALA:HB3 | 2.01                     | 0.61              |
| 27:BA:244:A:O2'    | 38:BP:73:GLY:CA   | 2.49                     | 0.61              |
| 1:CA:250:A:H1'     | 1:CA:252:U:C5     | 2.35                     | 0.61              |
| 1:CA:284:G:H2'     | 1:CA:285:G:C8     | 2.30                     | 0.61              |
| 1:CA:339:C:H2'     | 1:CA:340:U:H6     | 1.65                     | 0.61              |
| 1:CA:928:G:H1      | 1:CA:1389:C:H42   | 1.49                     | 0.61              |
| 2:CB:134:GLU:HA    | 2:CB:137:ARG:HB3  | 1.83                     | 0.61              |
| 8:CH:109:ILE:HG22  | 8:CH:137:VAL:O    | 2.00                     | 0.61              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 11:CK:13:GLN:NE2    | 11:CK:75:TYR:HA   | 2.15                     | 0.61              |
| 17:CQ:27:PHE:CD2    | 17:CQ:27:PHE:N    | 2.68                     | 0.61              |
| 20:CT:22:ARG:O      | 20:CT:26:ASN:ND2  | 2.33                     | 0.61              |
| 26:CZ:4:SER:C       | 26:CZ:5:UAL:H6    | 2.01                     | 0.61              |
| 53:D4:42:CYS:SG     | 53:D4:46:ASN:HB3  | 2.40                     | 0.61              |
| 27:DA:1247:A:O2'    | 27:DA:1248:G:H5'' | 2.01                     | 0.61              |
| 27:DA:1299:G:H5''   | 27:DA:1300:U:OP1  | 2.01                     | 0.61              |
| 27:DA:1952:A:C6     | 37:DO:22:ILE:HD12 | 2.35                     | 0.61              |
| 27:DA:2197:U:HO2'   | 27:DA:2198:A:H2'  | 1.64                     | 0.61              |
| 27:DA:663:G:H2'     | 27:DA:664:C:C6    | 2.36                     | 0.61              |
| 27:DA:746:A:H1'     | 27:DA:748:G:N2    | 2.14                     | 0.61              |
| 27:DA:875:G:H2'     | 27:DA:876:C:C6    | 2.36                     | 0.61              |
| 30:DD:27:THR:CG2    | 30:DD:83:GLU:HG2  | 2.29                     | 0.61              |
| 34:DH:92:ILE:HG22   | 34:DH:93:GLY:N    | 2.14                     | 0.61              |
| 36:DN:10:GLU:OE2    | 36:DN:11:PRO:HD2  | 2.00                     | 0.61              |
| 37:DO:11:ALA:O      | 37:DO:98:VAL:HA   | 2.01                     | 0.61              |
| 38:DP:121:LYS:O     | 38:DP:123:LEU:HG  | 2.00                     | 0.61              |
| 46:DX:44:GLU:O      | 46:DX:46:ALA:N    | 2.33                     | 0.61              |
| 47:DY:45:VAL:HA     | 47:DY:62:GLU:HG2  | 1.82                     | 0.61              |
| 1:AA:1070:U:H2'     | 1:AA:1071:C:C6    | 2.36                     | 0.61              |
| 1:AA:575:G:H4'      | 1:AA:576:G:O5'    | 2.00                     | 0.61              |
| 16:AP:14:ASN:HA     | 16:AP:42:ARG:NH2  | 2.16                     | 0.61              |
| 16:AP:20:VAL:CG2    | 16:AP:21:VAL:N    | 2.63                     | 0.61              |
| 18:AR:66:LEU:HD11   | 18:AR:70:ILE:HD11 | 1.82                     | 0.61              |
| 19:AS:44:MET:O      | 19:AS:62:ILE:HG12 | 2.00                     | 0.61              |
| 23:AW:6:U:C2'       | 23:AW:7:A:H5''    | 2.30                     | 0.61              |
| 24:AX:50:U:H3       | 24:AX:64:G:H1     | 1.49                     | 0.61              |
| 27:BA:2277:G:OP2    | 49:B0:12:ASN:OD1  | 2.18                     | 0.61              |
| 49:B0:21:LEU:HD22   | 49:B0:39:ARG:HB3  | 1.83                     | 0.61              |
| 27:BA:1344:G:H5'    | 27:BA:1384:A:N6   | 2.16                     | 0.61              |
| 27:BA:1445(A):C:H2' | 27:BA:1446:C:H6   | 1.65                     | 0.61              |
| 27:BA:2306:C:H5'    | 27:BA:2307:G:O4'  | 2.01                     | 0.61              |
| 27:BA:480:A:H2      | 27:BA:499:U:O2    | 1.83                     | 0.61              |
| 27:BA:60:G:C5       | 27:BA:63:U:C4     | 2.89                     | 0.61              |
| 27:BA:686:G:H4'     | 27:BA:687:C:OP2   | 1.98                     | 0.61              |
| 27:BA:703:U:H2'     | 27:BA:704:G:H5'   | 1.82                     | 0.61              |
| 27:BA:892:G:H2'     | 27:BA:892:G:N3    | 2.16                     | 0.61              |
| 30:BD:142:VAL:HG23  | 30:BD:192:THR:O   | 2.00                     | 0.61              |
| 30:BD:68:LYS:HG3    | 30:BD:68:LYS:O    | 2.01                     | 0.61              |
| 31:BE:167:VAL:HG13  | 31:BE:189:PRO:HD3 | 1.83                     | 0.61              |
| 32:BF:136:THR:O     | 32:BF:140:LEU:HB2 | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BP:10:PRO:O    | 38:BP:11:GLY:O    | 2.19                     | 0.61              |
| 39:BQ:43:THR:HG22 | 39:BQ:94:VAL:HG12 | 1.83                     | 0.61              |
| 39:BQ:39:PRO:HD3  | 39:BQ:99:PRO:CG   | 2.30                     | 0.61              |
| 40:BR:18:LEU:O    | 40:BR:18:LEU:HD13 | 2.01                     | 0.61              |
| 40:BR:96:ARG:HG2  | 40:BR:97:VAL:N    | 2.16                     | 0.61              |
| 46:BX:26:TYR:CD2  | 46:BX:92:LEU:HD12 | 2.35                     | 0.61              |
| 2:CB:236:TYR:HD2  | 2:CB:239:VAL:HB   | 1.65                     | 0.61              |
| 4:CD:76:ARG:O     | 4:CD:79:PHE:N     | 2.34                     | 0.61              |
| 5:CE:13:ILE:HG23  | 5:CE:29:GLY:O     | 2.01                     | 0.61              |
| 50:D1:46:LEU:C    | 50:D1:47:GLN:HE21 | 2.04                     | 0.61              |
| 27:DA:1655:A:H4'  | 31:DE:114:ALA:CA  | 2.31                     | 0.61              |
| 27:DA:1649:G:N1   | 27:DA:2009:G:C6   | 2.69                     | 0.61              |
| 27:DA:2261:C:H5'  | 27:DA:2388:A:H4'  | 1.83                     | 0.61              |
| 27:DA:2838:G:H1'  | 40:DR:45:ARG:HH11 | 1.64                     | 0.61              |
| 27:DA:671:C:O2'   | 27:DA:672:C:O5'   | 2.19                     | 0.61              |
| 27:DA:859:G:H21   | 27:DA:916:G:H2'   | 1.66                     | 0.61              |
| 27:DA:957:A:N6    | 27:DA:959:A:C2    | 2.69                     | 0.61              |
| 30:DD:10:THR:HG23 | 30:DD:13:ARG:CB   | 2.29                     | 0.61              |
| 30:DD:69:ARG:HH12 | 30:DD:192:THR:HB  | 1.65                     | 0.61              |
| 31:DE:91:VAL:HG12 | 31:DE:92:THR:H    | 1.64                     | 0.61              |
| 33:DG:16:ARG:N    | 33:DG:17:PRO:HD2  | 2.16                     | 0.61              |
| 33:DG:51:ARG:CZ   | 33:DG:51:ARG:HA   | 2.30                     | 0.61              |
| 34:DH:104:GLU:HA  | 34:DH:113:VAL:O   | 2.01                     | 0.61              |
| 34:DH:156:ALA:C   | 34:DH:158:HIS:N   | 2.52                     | 0.61              |
| 39:DQ:137:TYR:OH  | 48:DZ:80:ARG:NH2  | 2.32                     | 0.61              |
| 42:DT:62:THR:HG22 | 42:DT:75:ILE:HG12 | 1.82                     | 0.61              |
| 44:DV:62:LEU:HD21 | 44:DV:95:LEU:N    | 2.15                     | 0.61              |
| 47:DY:9:LYS:O     | 47:DY:11:ASP:N    | 2.34                     | 0.61              |
| 48:DZ:41:VAL:O    | 48:DZ:45:LYS:HG3  | 2.00                     | 0.61              |
| 1:AA:1428:A:H2'   | 1:AA:1429:C:C6    | 2.36                     | 0.61              |
| 1:AA:666:G:O2'    | 1:AA:667:G:H5'    | 2.01                     | 0.61              |
| 1:AA:822:C:O2'    | 1:AA:823:G:H5'    | 2.01                     | 0.61              |
| 2:AB:17:PHE:CD2   | 2:AB:17:PHE:N     | 2.68                     | 0.61              |
| 3:AC:150:LYS:HE3  | 3:AC:167:TRP:NE1  | 2.14                     | 0.61              |
| 3:AC:152:ILE:O    | 3:AC:198:VAL:HG12 | 2.00                     | 0.61              |
| 7:AG:26:PHE:CD1   | 7:AG:101:LEU:HD22 | 2.35                     | 0.61              |
| 12:AL:38:ARG:HH22 | 12:AL:54:LYS:HZ3  | 1.48                     | 0.61              |
| 14:AN:27:CYS:O    | 14:AN:27:CYS:SG   | 2.59                     | 0.61              |
| 27:BA:97:C:H5''   | 51:B2:2:LYS:CB    | 2.30                     | 0.61              |
| 57:B8:32:LEU:HB3  | 57:B8:36:LYS:HD2  | 1.83                     | 0.61              |
| 27:BA:1839:G:H2'  | 27:BA:1840:G:H8   | 1.66                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1996:C:H4'  | 27:BA:1997:G:O5'   | 2.00                     | 0.61              |
| 27:BA:2533:A:C3'  | 27:BA:2534:A:H5''  | 2.31                     | 0.61              |
| 27:BA:2809:A:O2'  | 27:BA:2810:A:H5'   | 1.99                     | 0.61              |
| 27:BA:386:G:O2'   | 27:BA:387:U:OP1    | 2.16                     | 0.61              |
| 27:BA:470:A:H2'   | 27:BA:471:A:C8     | 2.36                     | 0.61              |
| 27:BA:500:G:N2    | 27:BA:503:A:C8     | 2.69                     | 0.61              |
| 27:BA:587:C:O2'   | 27:BA:588:U:OP2    | 2.17                     | 0.61              |
| 27:BA:715:G:H2'   | 27:BA:716:A:C8     | 2.36                     | 0.61              |
| 29:BC:77:ILE:O    | 29:BC:77:ILE:HG23  | 2.00                     | 0.61              |
| 30:BD:27:THR:HG23 | 30:BD:27:THR:O     | 1.99                     | 0.61              |
| 34:BH:70:THR:O    | 34:BH:72:ILE:N     | 2.34                     | 0.61              |
| 38:BP:85:LEU:HD23 | 38:BP:85:LEU:N     | 2.16                     | 0.61              |
| 42:BT:23:ARG:HA   | 42:BT:52:ILE:HD12  | 1.83                     | 0.61              |
| 36:BN:40:PRO:O    | 43:BU:64:ARG:HD3   | 2.01                     | 0.61              |
| 46:BX:14:SER:O    | 46:BX:17:ALA:N     | 2.33                     | 0.61              |
| 39:BQ:134:ARG:NH2 | 48:BZ:121:ARG:CZ   | 2.61                     | 0.61              |
| 1:CA:276:G:C2'    | 1:CA:277:C:H5'     | 2.31                     | 0.61              |
| 1:CA:344:A:O2'    | 1:CA:345:C:OP1     | 2.17                     | 0.61              |
| 1:CA:961:U:O2'    | 1:CA:962:C:H6      | 1.83                     | 0.61              |
| 2:CB:80:ILE:HD13  | 2:CB:211:ILE:HG22  | 1.83                     | 0.61              |
| 3:CC:27:LYS:HB3   | 3:CC:27:LYS:NZ     | 2.16                     | 0.61              |
| 6:CF:21:LEU:O     | 6:CF:24:GLU:HG2    | 2.00                     | 0.61              |
| 16:CP:31:LYS:HG2  | 16:CP:32:TYR:N     | 2.16                     | 0.61              |
| 17:CQ:50:LYS:HE2  | 17:CQ:51:TYR:CE1   | 2.36                     | 0.61              |
| 24:CX:37:A:H3'    | 24:CX:38:A:C8      | 2.35                     | 0.61              |
| 27:DA:1252:G:C8   | 27:DA:1252:G:OP1   | 2.54                     | 0.61              |
| 27:DA:2103:C:H3'  | 27:DA:2104:G:H5''  | 1.82                     | 0.61              |
| 27:DA:2306:C:H5'  | 27:DA:2307:G:O5'   | 2.01                     | 0.61              |
| 27:DA:2362:G:O2'  | 27:DA:2363:C:H5'   | 2.01                     | 0.61              |
| 27:DA:627:A:H4'   | 27:DA:628:G:OP1    | 2.00                     | 0.61              |
| 27:DA:733:G:H8    | 27:DA:733:G:O5'    | 1.84                     | 0.61              |
| 27:DA:744:G:OP1   | 31:DE:132:HIS:HB3  | 2.01                     | 0.61              |
| 28:DB:24:G:N3     | 28:DB:27:C:N4      | 2.48                     | 0.61              |
| 30:DD:69:ARG:NH1  | 30:DD:192:THR:HB   | 2.15                     | 0.61              |
| 34:DH:135:GLY:HA3 | 34:DH:141:VAL:HG22 | 1.83                     | 0.61              |
| 36:DN:114:ARG:O   | 36:DN:117:PHE:HB3  | 2.01                     | 0.61              |
| 40:DR:11:ASN:HB3  | 40:DR:12:ARG:HH11  | 1.64                     | 0.61              |
| 31:DE:111:ARG:CA  | 40:DR:2:ARG:HG3    | 2.29                     | 0.61              |
| 41:DS:101:LEU:CD1 | 41:DS:101:LEU:H    | 2.14                     | 0.61              |
| 48:DZ:54:HIS:NE2  | 48:DZ:134:GLU:HG3  | 2.15                     | 0.61              |
| 1:AA:376:G:H5''   | 16:AP:5:ARG:CB     | 2.25                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:533:A:HO2'   | 1:AA:534:U:H5''   | 1.65                     | 0.60              |
| 2:AB:155:LEU:HD12 | 2:AB:159:PRO:HD3  | 1.83                     | 0.60              |
| 1:AA:403:C:H5''   | 4:AD:136:PRO:HD2  | 1.83                     | 0.60              |
| 4:AD:159:ARG:HH11 | 4:AD:159:ARG:HG3  | 1.65                     | 0.60              |
| 5:AE:78:HIS:CE1   | 5:AE:142:LEU:HA   | 2.36                     | 0.60              |
| 8:AH:42:GLU:OE2   | 8:AH:120:THR:HG21 | 2.00                     | 0.60              |
| 13:AM:102:ARG:HG3 | 13:AM:102:ARG:NH1 | 2.15                     | 0.60              |
| 23:AW:63:C:H2'    | 23:AW:64:G:C8     | 2.35                     | 0.60              |
| 27:BA:250:G:OP2   | 57:B8:13:ARG:NH2  | 2.33                     | 0.60              |
| 57:B8:44:LYS:N    | 57:B8:44:LYS:HD2  | 2.15                     | 0.60              |
| 27:BA:1598:C:O2   | 27:BA:1598:C:H2'  | 2.01                     | 0.60              |
| 27:BA:1799:G:H4'  | 27:BA:1800:C:O5'  | 2.01                     | 0.60              |
| 27:BA:1922:G:H2'  | 27:BA:1923:U:C6   | 2.36                     | 0.60              |
| 27:BA:2036:C:H6   | 27:BA:2036:C:H5'  | 1.66                     | 0.60              |
| 27:BA:345:A:N3    | 27:BA:347:A:N6    | 2.49                     | 0.60              |
| 27:BA:581:C:O2'   | 27:BA:582:G:H5'   | 2.01                     | 0.60              |
| 27:BA:635:C:H2'   | 27:BA:636:G:H8    | 1.66                     | 0.60              |
| 38:BP:70:GLN:HA   | 38:BP:70:GLN:OE1  | 2.02                     | 0.60              |
| 42:BT:129:ARG:O   | 42:BT:129:ARG:HG3 | 2.01                     | 0.60              |
| 42:BT:68:TYR:HD2  | 42:BT:68:TYR:N    | 1.99                     | 0.60              |
| 44:BV:39:LEU:HA   | 44:BV:47:VAL:HG11 | 1.83                     | 0.60              |
| 48:BZ:107:PRO:CD  | 48:BZ:116:LEU:HB2 | 2.31                     | 0.60              |
| 1:CA:1286:A:C8    | 1:CA:1287:A:H4'   | 2.36                     | 0.60              |
| 1:CA:1459:C:O2'   | 1:CA:1460:A:H5'   | 2.00                     | 0.60              |
| 1:CA:787:A:H2     | 1:CA:795:C:H41    | 1.47                     | 0.60              |
| 5:CE:101:ILE:HG13 | 5:CE:119:LEU:HD23 | 1.81                     | 0.60              |
| 5:CE:33:VAL:HG22  | 5:CE:43:LEU:CD1   | 2.31                     | 0.60              |
| 6:CF:43:LEU:O     | 6:CF:44:GLY:O     | 2.19                     | 0.60              |
| 9:CI:55:ALA:CB    | 9:CI:59:PHE:HE1   | 2.14                     | 0.60              |
| 10:CJ:45:ARG:HB3  | 10:CJ:65:LEU:HB3  | 1.82                     | 0.60              |
| 10:CJ:81:THR:O    | 10:CJ:83:GLU:N    | 2.32                     | 0.60              |
| 23:CW:63:C:H2'    | 23:CW:64:G:C8     | 2.36                     | 0.60              |
| 27:DA:1962:C:O2'  | 27:DA:1964:G:OP2  | 2.17                     | 0.60              |
| 27:DA:2223:G:H2'  | 27:DA:2224:G:C5'  | 2.27                     | 0.60              |
| 27:DA:2569:G:C2'  | 27:DA:2570:G:H5'  | 2.32                     | 0.60              |
| 27:DA:720:C:H2'   | 27:DA:721:C:H6    | 1.65                     | 0.60              |
| 27:DA:953:A:H2'   | 27:DA:954:G:H8    | 1.65                     | 0.60              |
| 27:DA:2758:A:C5   | 34:DH:67:LEU:HD21 | 2.35                     | 0.60              |
| 39:DQ:81:VAL:HG22 | 39:DQ:82:ARG:N    | 2.16                     | 0.60              |
| 27:DA:2838:G:C1'  | 40:DR:45:ARG:NH1  | 2.59                     | 0.60              |
| 43:DU:112:ARG:O   | 43:DU:115:ALA:HB3 | 2.00                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:DU:68:ALA:O     | 43:DU:71:GLN:HG3   | 2.01                     | 0.60              |
| 44:DV:58:VAL:HG12  | 44:DV:59:ALA:N     | 2.16                     | 0.60              |
| 48:DZ:140:VAL:HG23 | 48:DZ:143:LEU:HD23 | 1.83                     | 0.60              |
| 1:AA:1054:C:C5     | 1:AA:1196:U:H2'    | 2.36                     | 0.60              |
| 1:AA:1081:G:O2'    | 1:AA:1082:G:H5'    | 2.01                     | 0.60              |
| 1:AA:489:C:H2'     | 1:AA:490:G:C8      | 2.36                     | 0.60              |
| 1:AA:594:G:H2'     | 1:AA:595:G:H5'     | 1.81                     | 0.60              |
| 2:AB:70:PHE:O      | 2:AB:93:VAL:HG22   | 2.01                     | 0.60              |
| 10:AJ:90:LEU:H     | 10:AJ:91:PRO:CD    | 2.14                     | 0.60              |
| 11:AK:126:ARG:C    | 11:AK:128:ALA:H    | 2.01                     | 0.60              |
| 55:B6:51:GLU:O     | 55:B6:52:VAL:CB    | 2.48                     | 0.60              |
| 27:BA:1204:A:N6    | 27:BA:1240:U:H2'   | 2.16                     | 0.60              |
| 27:BA:2462:U:H3    | 27:BA:2488:A:N6    | 1.97                     | 0.60              |
| 27:BA:2790:A:C2    | 27:BA:2791:C:H3'   | 2.27                     | 0.60              |
| 27:BA:1971:A:C4    | 30:BD:241:PRO:HG3  | 2.36                     | 0.60              |
| 36:BN:113:GLY:O    | 36:BN:116:LEU:HB2  | 2.02                     | 0.60              |
| 40:BR:12:ARG:HD3   | 40:BR:16:HIS:CG    | 2.36                     | 0.60              |
| 41:BS:15:ARG:C     | 41:BS:17:ARG:O     | 2.38                     | 0.60              |
| 44:BV:91:TYR:O     | 44:BV:92:THR:HG22  | 2.00                     | 0.60              |
| 45:BW:73:ALA:HB3   | 45:BW:106:ILE:HG12 | 1.81                     | 0.60              |
| 48:BZ:107:PRO:C    | 48:BZ:109:GLY:H    | 2.03                     | 0.60              |
| 1:CA:181:G:H21     | 1:CA:183:G:N2      | 1.98                     | 0.60              |
| 1:CA:286:G:O2'     | 1:CA:287:U:H5'     | 1.99                     | 0.60              |
| 1:CA:538:G:O2'     | 1:CA:539:A:H5'     | 2.01                     | 0.60              |
| 2:CB:178:ARG:HH22  | 8:CH:74:PRO:HG3    | 1.67                     | 0.60              |
| 3:CC:190:ARG:HG2   | 3:CC:190:ARG:HH11  | 1.66                     | 0.60              |
| 19:CS:38:SER:O     | 19:CS:70:LYS:HB3   | 2.00                     | 0.60              |
| 27:DA:1430:C:H2'   | 27:DA:1431:U:H6    | 1.66                     | 0.60              |
| 27:DA:1785:A:OP2   | 27:DA:1982:C:H5'   | 2.01                     | 0.60              |
| 27:DA:1904:G:O2'   | 27:DA:1905:C:H5'   | 2.01                     | 0.60              |
| 27:DA:2715:C:H2'   | 27:DA:2716:U:C6    | 2.36                     | 0.60              |
| 27:DA:324:A:H2'    | 27:DA:325:G:O4'    | 2.02                     | 0.60              |
| 27:DA:17:G:H1      | 27:DA:523:C:H42    | 1.49                     | 0.60              |
| 27:DA:632:A:H2'    | 27:DA:633:A:C8     | 2.37                     | 0.60              |
| 27:DA:887:A:C2'    | 27:DA:888:C:H5''   | 2.31                     | 0.60              |
| 30:DD:267:SER:O    | 30:DD:268:ARG:CB   | 2.50                     | 0.60              |
| 30:DD:43:ARG:HB2   | 30:DD:54:ARG:CB    | 2.32                     | 0.60              |
| 31:DE:102:VAL:HG22 | 31:DE:170:LEU:O    | 2.00                     | 0.60              |
| 36:DN:15:LEU:HD12  | 36:DN:136:GLU:CG   | 2.29                     | 0.60              |
| 46:DX:26:TYR:CD1   | 46:DX:89:ILE:HD12  | 2.35                     | 0.60              |
| 48:DZ:119:ILE:O    | 48:DZ:170:ILE:HA   | 2.02                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:DZ:75:LEU:HA    | 48:DZ:82:PRO:HA    | 1.82                     | 0.60              |
| 1:AA:1001(A):G:C8  | 1:AA:1002:G:H8     | 2.20                     | 0.60              |
| 1:AA:1292:U:H2'    | 1:AA:1293:G:C8     | 2.37                     | 0.60              |
| 1:AA:1306:A:N6     | 1:AA:1331:G:H1'    | 2.16                     | 0.60              |
| 1:AA:1452:C:H4'    | 1:AA:1456:G:C2     | 2.36                     | 0.60              |
| 1:AA:865:A:H2      | 1:AA:918:A:H4'     | 1.66                     | 0.60              |
| 3:AC:156:ARG:H     | 3:AC:163:ALA:HA    | 1.66                     | 0.60              |
| 4:AD:141:ARG:N     | 4:AD:144:ASP:OD2   | 2.33                     | 0.60              |
| 16:AP:23:ASP:O     | 16:AP:24:ALA:C     | 2.40                     | 0.60              |
| 1:AA:390:C:O3'     | 16:AP:28:ARG:NH2   | 2.34                     | 0.60              |
| 19:AS:41:VAL:O     | 19:AS:44:MET:HB2   | 2.01                     | 0.60              |
| 27:BA:2346:A:H8    | 27:BA:2383:G:C5    | 2.17                     | 0.60              |
| 27:BA:252:G:H2'    | 27:BA:253:C:H6     | 1.66                     | 0.60              |
| 27:BA:2876:G:H4'   | 42:BT:3:ARG:HD2    | 1.81                     | 0.60              |
| 27:BA:707:G:H5'    | 27:BA:708:C:OP2    | 2.00                     | 0.60              |
| 28:BB:57:A:C4      | 33:BG:29:TRP:HB2   | 2.37                     | 0.60              |
| 31:BE:35:GLN:HE21  | 31:BE:37:ARG:HD3   | 1.66                     | 0.60              |
| 34:BH:85:LYS:HD2   | 34:BH:141:VAL:HG13 | 1.81                     | 0.60              |
| 35:BI:82:ARG:CB    | 35:BI:82:ARG:HH11  | 2.12                     | 0.60              |
| 38:BP:7:ARG:O      | 38:BP:10:PRO:CD    | 2.49                     | 0.60              |
| 41:BS:101:LEU:HD13 | 41:BS:101:LEU:O    | 2.01                     | 0.60              |
| 43:BU:8:VAL:HG12   | 43:BU:9:VAL:N      | 2.16                     | 0.60              |
| 47:BY:97:ARG:O     | 47:BY:98:VAL:HG23  | 2.01                     | 0.60              |
| 1:CA:1046:A:H3'    | 1:CA:1047:G:H8     | 1.66                     | 0.60              |
| 1:CA:1053:G:N7     | 1:CA:1199:U:H3'    | 2.16                     | 0.60              |
| 1:CA:327:A:O2'     | 1:CA:329:A:H5'     | 2.02                     | 0.60              |
| 1:CA:500:G:H2'     | 1:CA:501:C:H6      | 1.65                     | 0.60              |
| 1:CA:580:U:H2'     | 1:CA:581:G:C8      | 2.36                     | 0.60              |
| 1:CA:862:C:C1'     | 1:CA:874:G:H4'     | 2.31                     | 0.60              |
| 4:CD:33:MET:HE3    | 4:CD:33:MET:HA     | 1.83                     | 0.60              |
| 1:CA:406:G:C5'     | 4:CD:5:ILE:HG21    | 2.32                     | 0.60              |
| 4:CD:9:CYS:SG      | 4:CD:22:LYS:CD     | 2.78                     | 0.60              |
| 3:CC:135:LYS:NZ    | 5:CE:53:LEU:HD21   | 2.15                     | 0.60              |
| 6:CF:97:PHE:CD2    | 18:CR:65:ILE:HD13  | 2.36                     | 0.60              |
| 12:CL:24:LEU:HG    | 12:CL:59:SER:CB    | 2.32                     | 0.60              |
| 20:CT:84:LEU:O     | 20:CT:88:VAL:HG23  | 2.01                     | 0.60              |
| 27:DA:1017:G:O2'   | 27:DA:1018:C:H5'   | 2.00                     | 0.60              |
| 27:DA:1022:G:O2'   | 27:DA:1024:G:N7    | 2.30                     | 0.60              |
| 27:DA:1569:A:H1'   | 30:DD:38:LYS:NZ    | 2.16                     | 0.60              |
| 27:DA:1688:U:H1'   | 27:DA:1701:A:C6    | 2.36                     | 0.60              |
| 27:DA:1788:C:O2'   | 27:DA:1789:A:H5'   | 2.01                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2087:G:C6    | 27:DA:2233:U:N3    | 2.68                     | 0.60              |
| 27:DA:2586:C:O2'   | 27:DA:2587:A:H5'   | 2.02                     | 0.60              |
| 27:DA:2752:C:C2'   | 27:DA:2753:A:H8    | 2.13                     | 0.60              |
| 27:DA:324:A:O2'    | 27:DA:325:G:H5'    | 2.02                     | 0.60              |
| 27:DA:372:G:N2     | 27:DA:400:G:H2'    | 2.16                     | 0.60              |
| 27:DA:391:G:O5'    | 27:DA:391:G:H8     | 1.83                     | 0.60              |
| 28:DB:31:C:H2'     | 28:DB:53:A:H61     | 1.67                     | 0.60              |
| 30:DD:147:LEU:O    | 30:DD:189:CYS:SG   | 2.53                     | 0.60              |
| 31:DE:128:SER:O    | 31:DE:129:HIS:HB2  | 2.00                     | 0.60              |
| 37:DO:103:ALA:HA   | 37:DO:122:LEU:O    | 2.02                     | 0.60              |
| 46:DX:5:TYR:N      | 46:DX:5:TYR:CD1    | 2.69                     | 0.60              |
| 1:AA:823:G:H21     | 8:AH:1:MET:CE      | 2.15                     | 0.60              |
| 1:AA:640:A:H2      | 8:AH:115:SER:HB3   | 1.65                     | 0.60              |
| 16:AP:18:ARG:O     | 16:AP:20:VAL:HG12  | 2.01                     | 0.60              |
| 19:AS:51:VAL:O     | 19:AS:58:VAL:HG22  | 2.02                     | 0.60              |
| 25:AY:17:G:H22     | 25:AY:54:U:H1'     | 1.66                     | 0.60              |
| 50:B1:5:CYS:HG     | 50:B1:8:SER:HG     | 1.49                     | 0.60              |
| 51:B2:15:LYS:O     | 51:B2:16:LEU:HD23  | 2.01                     | 0.60              |
| 27:BA:121:G:C8     | 27:BA:121:G:H5''   | 2.36                     | 0.60              |
| 27:BA:2839:G:H2'   | 27:BA:2840:C:H6    | 1.66                     | 0.60              |
| 27:BA:361:G:H2'    | 27:BA:362:U:H5''   | 1.82                     | 0.60              |
| 28:BB:105:A:H2'    | 28:BB:106:G:H5'    | 1.83                     | 0.60              |
| 31:BE:143:ASN:OD1  | 31:BE:147:PRO:HD2  | 2.02                     | 0.60              |
| 33:BG:111:LEU:HD23 | 33:BG:114:ILE:HD12 | 1.84                     | 0.60              |
| 34:BH:43:VAL:CB    | 34:BH:52:VAL:HA    | 2.32                     | 0.60              |
| 34:BH:97:ARG:HG2   | 34:BH:98:LEU:N     | 2.15                     | 0.60              |
| 35:BI:45:LYS:O     | 35:BI:48:GLU:HB2   | 2.01                     | 0.60              |
| 36:BN:34:LEU:O     | 36:BN:49:GLY:HA3   | 2.00                     | 0.60              |
| 36:BN:16:ILE:O     | 36:BN:54:VAL:HA    | 2.02                     | 0.60              |
| 37:BO:97:ARG:HB3   | 37:BO:99:PHE:CE1   | 2.36                     | 0.60              |
| 43:BU:83:LEU:HD13  | 43:BU:113:ALA:HB2  | 1.82                     | 0.60              |
| 1:CA:1396:A:H4'    | 1:CA:1397:C:H5'    | 1.82                     | 0.60              |
| 1:CA:560:U:H4'     | 1:CA:561:U:OP2     | 2.01                     | 0.60              |
| 1:CA:885:G:N3      | 1:CA:914:A:C2      | 2.69                     | 0.60              |
| 1:CA:963:G:H21     | 10:CJ:55:LYS:NZ    | 1.98                     | 0.60              |
| 3:CC:150:LYS:HB3   | 3:CC:201:TYR:HB2   | 1.83                     | 0.60              |
| 3:CC:89:GLU:O      | 3:CC:93:LYS:HB2    | 2.02                     | 0.60              |
| 5:CE:105:VAL:HB    | 5:CE:106:PRO:CD    | 2.31                     | 0.60              |
| 8:CH:11:THR:HG22   | 8:CH:15:ASN:HD21   | 1.65                     | 0.60              |
| 13:CM:22:ILE:CG2   | 13:CM:25:ILE:HD13  | 2.31                     | 0.60              |
| 15:CO:37:ASN:H     | 15:CO:37:ASN:ND2   | 1.98                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:CS:32:LYS:HB3   | 19:CS:57:HIS:CD2   | 2.36                     | 0.60              |
| 23:CW:18:G:H1'     | 23:CW:19:U:N3      | 2.16                     | 0.60              |
| 27:DA:517:C:OP1    | 54:D5:16:ARG:NH2   | 2.34                     | 0.60              |
| 27:DA:1231:G:O2'   | 27:DA:1232:G:H5'   | 2.01                     | 0.60              |
| 27:DA:1884:A:H2'   | 27:DA:1885:A:C5'   | 2.22                     | 0.60              |
| 27:DA:195:A:OP1    | 38:DP:46:LYS:HE2   | 2.01                     | 0.60              |
| 27:DA:2525:G:N2    | 27:DA:2539:C:C2    | 2.69                     | 0.60              |
| 27:DA:2848:G:H1'   | 27:DA:2867:G:N2    | 2.16                     | 0.60              |
| 27:DA:316:C:O5'    | 27:DA:316:C:H6     | 1.85                     | 0.60              |
| 27:DA:662:G:P      | 38:DP:18:ARG:HD2   | 2.41                     | 0.60              |
| 30:DD:227:ASN:HB3  | 30:DD:228:PRO:HD2  | 1.82                     | 0.60              |
| 35:DI:44:LEU:O     | 35:DI:47:LEU:HB3   | 2.01                     | 0.60              |
| 36:DN:18:ALA:HB1   | 36:DN:21:LYS:CB    | 2.31                     | 0.60              |
| 40:DR:2:ARG:NH2    | 40:DR:5:LYS:NZ     | 2.50                     | 0.60              |
| 47:DY:96:ILE:HG13  | 47:DY:99:CYS:HB2   | 1.83                     | 0.60              |
| 48:DZ:127:VAL:HG22 | 48:DZ:128:SER:N    | 2.09                     | 0.60              |
| 48:DZ:27:MET:HE3   | 48:DZ:32:LEU:HD11  | 1.83                     | 0.60              |
| 1:AA:1074:G:H2'    | 1:AA:1075:C:C6     | 2.37                     | 0.60              |
| 1:AA:1406:U:C2'    | 1:AA:1407:C:H5'    | 2.32                     | 0.60              |
| 1:AA:1499:A:H1'    | 1:AA:1520:G:H5'    | 1.83                     | 0.60              |
| 1:AA:232:G:H2'     | 1:AA:233:C:H6      | 1.67                     | 0.60              |
| 3:AC:182:ILE:HG12  | 3:AC:203:PHE:HA    | 1.82                     | 0.60              |
| 6:AF:43:LEU:N      | 6:AF:43:LEU:HD12   | 2.05                     | 0.60              |
| 7:AG:113:GLU:HG3   | 7:AG:119:ARG:HG2   | 1.84                     | 0.60              |
| 9:AI:26:VAL:HB     | 9:AI:33:PHE:HB2    | 1.84                     | 0.60              |
| 12:AL:50:ARG:HG2   | 12:AL:50:ARG:HH11  | 1.67                     | 0.60              |
| 13:AM:102:ARG:HG3  | 13:AM:102:ARG:HH11 | 1.67                     | 0.60              |
| 13:AM:8:GLU:OE1    | 13:AM:22:ILE:HG12  | 2.01                     | 0.60              |
| 19:AS:61:TYR:O     | 19:AS:62:ILE:HB    | 2.01                     | 0.60              |
| 23:AW:62:U:O2'     | 27:BA:2482:G:H4'   | 2.00                     | 0.60              |
| 49:B0:41:ARG:O     | 49:B0:57:PHE:CD2   | 2.54                     | 0.60              |
| 27:BA:1036:G:O2'   | 27:BA:1037:G:H5'   | 2.02                     | 0.60              |
| 27:BA:1815:A:P     | 30:BD:54:ARG:HH12  | 2.24                     | 0.60              |
| 33:BG:56:ALA:HB2   | 33:BG:153:ARG:HH21 | 1.66                     | 0.60              |
| 37:BO:71:ARG:HB3   | 37:BO:72:PRO:HD2   | 1.83                     | 0.60              |
| 42:BT:122:ASP:C    | 42:BT:124:ASP:N    | 2.54                     | 0.60              |
| 42:BT:28:VAL:O     | 42:BT:29:ARG:CB    | 2.48                     | 0.60              |
| 42:BT:60:THR:HG22  | 42:BT:77:PRO:HA    | 1.82                     | 0.60              |
| 43:BU:31:SER:C     | 43:BU:33:ARG:H     | 2.05                     | 0.60              |
| 1:CA:1056:U:O2'    | 1:CA:1057:G:H5'    | 2.02                     | 0.60              |
| 1:CA:223:U:O2'     | 1:CA:224:C:H5'     | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:882:C:O2'    | 1:CA:883:C:H5'    | 2.01                     | 0.60              |
| 4:CD:158:ILE:O    | 4:CD:162:LEU:HB2  | 2.02                     | 0.60              |
| 6:CF:12:PRO:HD2   | 6:CF:86:ARG:NH1   | 2.16                     | 0.60              |
| 6:CF:6:VAL:HG22   | 6:CF:90:VAL:HG13  | 1.82                     | 0.60              |
| 8:CH:38:ILE:HD13  | 8:CH:120:THR:HG22 | 1.84                     | 0.60              |
| 1:CA:973:G:O4'    | 10:CJ:55:LYS:HB3  | 2.00                     | 0.60              |
| 13:CM:8:GLU:OE2   | 13:CM:22:ILE:HA   | 2.01                     | 0.60              |
| 1:CA:192:U:C1'    | 20:CT:103:GLY:HA2 | 2.31                     | 0.60              |
| 27:DA:787:U:OP1   | 27:DA:1780:A:N6   | 2.34                     | 0.60              |
| 27:DA:1858:G:HO2' | 27:DA:1859:A:H8   | 1.49                     | 0.60              |
| 27:DA:639:U:H2'   | 27:DA:640:C:C6    | 2.36                     | 0.60              |
| 27:DA:675:A:C2'   | 27:DA:676:A:H5'   | 2.32                     | 0.60              |
| 27:DA:932:G:H4'   | 27:DA:933:A:O5'   | 2.01                     | 0.60              |
| 29:DC:58:VAL:HG21 | 29:DC:166:ASP:N   | 2.16                     | 0.60              |
| 35:DI:84:GLY:O    | 35:DI:85:GLU:HB2  | 2.00                     | 0.60              |
| 27:DA:2873:A:C2   | 40:DR:6:SER:HB3   | 2.36                     | 0.60              |
| 42:DT:35:LYS:O    | 42:DT:37:GLY:N    | 2.33                     | 0.60              |
| 45:DW:12:ILE:HG13 | 45:DW:42:ARG:NH1  | 2.17                     | 0.60              |
| 1:AA:1096:C:H2'   | 1:AA:1097:C:C6    | 2.36                     | 0.60              |
| 1:AA:1261:A:H2'   | 1:AA:1262:C:O4'   | 2.02                     | 0.60              |
| 1:AA:1484:C:O2'   | 1:AA:1485:U:H5'   | 2.02                     | 0.60              |
| 3:AC:64:VAL:O     | 3:AC:64:VAL:HG23  | 2.01                     | 0.60              |
| 5:AE:33:VAL:HG21  | 5:AE:109:ILE:CG1  | 2.31                     | 0.60              |
| 1:AA:939:G:H5''   | 7:AG:102:ARG:CZ   | 2.31                     | 0.60              |
| 10:AJ:80:LYS:HE3  | 10:AJ:80:LYS:C    | 2.22                     | 0.60              |
| 12:AL:74:LEU:HD21 | 12:AL:104:ALA:CB  | 2.32                     | 0.60              |
| 20:AT:41:ILE:HG13 | 20:AT:42:GLN:N    | 2.13                     | 0.60              |
| 54:B5:32:PRO:O    | 54:B5:33:CYS:HB3  | 2.01                     | 0.60              |
| 57:B8:52:LYS:N    | 57:B8:53:PRO:CD   | 2.65                     | 0.60              |
| 27:BA:1927:A:O2'  | 27:BA:1928:A:H5'  | 2.01                     | 0.60              |
| 27:BA:2133:G:H1'  | 27:BA:2158:A:H61  | 1.66                     | 0.60              |
| 27:BA:2695:C:H2'  | 27:BA:2696:U:C6   | 2.36                     | 0.60              |
| 27:BA:2699:C:O2'  | 27:BA:2700:C:H5'  | 2.01                     | 0.60              |
| 27:BA:2731:G:O5'  | 27:BA:2731:G:H8   | 1.84                     | 0.60              |
| 27:BA:31:C:H42    | 27:BA:474:G:H1    | 1.49                     | 0.60              |
| 27:BA:623:G:H2'   | 27:BA:624:C:H6    | 1.65                     | 0.60              |
| 27:BA:686:G:H2'   | 27:BA:788:A:N1    | 2.17                     | 0.60              |
| 32:BF:126:VAL:O   | 32:BF:127:GLU:HB2 | 2.01                     | 0.60              |
| 39:BQ:16:ARG:HG2  | 39:BQ:17:LEU:H    | 1.64                     | 0.60              |
| 40:BR:33:ARG:NE   | 40:BR:115:GLU:HB2 | 2.16                     | 0.60              |
| 40:BR:13:HIS:O    | 40:BR:14:SER:C    | 2.39                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BT:115:ARG:O   | 42:BT:116:ALA:HB2  | 2.01                     | 0.60              |
| 1:CA:1258:G:O2'   | 1:CA:1259:C:H5'    | 2.01                     | 0.60              |
| 1:CA:1445:C:H2'   | 1:CA:1446:U:H5'    | 1.84                     | 0.60              |
| 3:CC:64:VAL:CG2   | 3:CC:99:VAL:HA     | 2.31                     | 0.60              |
| 6:CF:82:ARG:HB2   | 6:CF:85:VAL:HG23   | 1.82                     | 0.60              |
| 13:CM:23:TYR:CE1  | 13:CM:70:LEU:HD23  | 2.36                     | 0.60              |
| 19:CS:13:ASP:O    | 19:CS:15:LEU:N     | 2.35                     | 0.60              |
| 27:DA:2357:U:OP1  | 49:D0:20:ARG:NH1   | 2.34                     | 0.60              |
| 55:D6:30:THR:HB   | 55:D6:31:PRO:CD    | 2.30                     | 0.60              |
| 27:DA:1343:G:O2'  | 27:DA:1344:G:H5'   | 2.02                     | 0.60              |
| 27:DA:151:C:C2'   | 27:DA:152:G:H5'    | 2.32                     | 0.60              |
| 27:DA:2750:A:H4'  | 27:DA:2751:G:OP1   | 2.01                     | 0.60              |
| 27:DA:48:G:H5'    | 27:DA:52:A:H4'     | 1.83                     | 0.60              |
| 27:DA:935:C:H2'   | 27:DA:936:C:C6     | 2.36                     | 0.60              |
| 32:DF:167:ALA:CB  | 32:DF:173:VAL:HG11 | 2.28                     | 0.60              |
| 37:DO:105:GLU:CA  | 37:DO:108:GLU:HG3  | 2.29                     | 0.60              |
| 38:DP:140:ALA:O   | 38:DP:141:ALA:HB3  | 2.01                     | 0.60              |
| 38:DP:6:LEU:HG    | 38:DP:9:ASN:ND2    | 2.16                     | 0.60              |
| 27:DA:29:U:C4'    | 43:DU:11:ARG:HH22  | 2.14                     | 0.60              |
| 27:DA:560:C:C4'   | 43:DU:52:ARG:HH22  | 2.13                     | 0.60              |
| 45:DW:47:VAL:O    | 45:DW:47:VAL:HG12  | 2.00                     | 0.60              |
| 46:DX:57:LEU:HD13 | 46:DX:78:LYS:O     | 2.02                     | 0.60              |
| 1:AA:198:G:H2'    | 1:AA:199:G:H8      | 1.66                     | 0.60              |
| 1:AA:861:G:O2'    | 1:AA:862:C:H5'     | 2.01                     | 0.60              |
| 5:AE:51:VAL:HB    | 5:AE:52:PRO:HD3    | 1.83                     | 0.60              |
| 8:AH:107:LEU:N    | 8:AH:107:LEU:HD23  | 2.17                     | 0.60              |
| 8:AH:2:LEU:CD1    | 8:AH:4:ASP:H       | 2.14                     | 0.60              |
| 17:AQ:56:VAL:O    | 17:AQ:76:LEU:HD12  | 2.01                     | 0.60              |
| 25:AY:52:G:O2'    | 25:AY:53:U:H5'     | 2.02                     | 0.60              |
| 27:BA:1150:C:C2'  | 27:BA:1151:G:H5'   | 2.32                     | 0.60              |
| 27:BA:2607:G:H2'  | 27:BA:2608:G:O4'   | 2.02                     | 0.60              |
| 27:BA:2667:C:H1'  | 34:BH:109:PHE:CE2  | 2.37                     | 0.60              |
| 27:BA:389:G:N1    | 38:BP:71:VAL:HG12  | 2.16                     | 0.60              |
| 27:BA:671:C:C5'   | 27:BA:671:C:H6     | 2.14                     | 0.60              |
| 27:BA:867:C:H2'   | 27:BA:868:U:C6     | 2.37                     | 0.60              |
| 27:BA:985:C:H2'   | 27:BA:986:C:H6     | 1.66                     | 0.60              |
| 31:BE:75:VAL:HG12 | 31:BE:76:ARG:N     | 2.17                     | 0.60              |
| 33:BG:44:GLY:H    | 33:BG:88:ILE:HD13  | 1.67                     | 0.60              |
| 38:BP:98:GLU:O    | 38:BP:101:VAL:HG22 | 2.01                     | 0.60              |
| 38:BP:84:ASN:HD22 | 38:BP:115:LEU:CG   | 2.13                     | 0.60              |
| 42:BT:98:LYS:HB3  | 42:BT:100:TYR:CE1  | 2.37                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BX:31:HIS:CD2   | 46:BX:32:PRO:HD2   | 2.37                     | 0.60              |
| 1:CA:1492:A:H3'    | 26:CZ:6:5OH:NP     | 2.16                     | 0.60              |
| 1:CA:47:C:O2'      | 1:CA:48:C:OP2      | 2.17                     | 0.60              |
| 1:CA:652:U:C1'     | 1:CA:653:A:H2      | 2.14                     | 0.60              |
| 1:CA:699:C:H2'     | 1:CA:700:G:H5'     | 1.84                     | 0.60              |
| 1:CA:714:G:O2'     | 1:CA:715:A:H5'     | 2.02                     | 0.60              |
| 1:CA:748:C:H4'     | 1:CA:749:C:O5'     | 2.01                     | 0.60              |
| 1:CA:803:G:O2'     | 1:CA:804:U:H5'     | 2.02                     | 0.60              |
| 3:CC:60:ALA:HB3    | 3:CC:63:ASN:OD1    | 2.02                     | 0.60              |
| 8:CH:9:MET:HB2     | 8:CH:26:VAL:HG21   | 1.84                     | 0.60              |
| 11:CK:50:TYR:CE2   | 11:CK:54:ARG:HD2   | 2.36                     | 0.60              |
| 12:CL:15:VAL:O     | 12:CL:16:ARG:HB3   | 2.01                     | 0.60              |
| 15:CO:3:ILE:O      | 15:CO:3:ILE:HG12   | 2.02                     | 0.60              |
| 21:CU:2:GLY:C      | 21:CU:4:GLY:N      | 2.55                     | 0.60              |
| 54:D5:16:ARG:NH1   | 54:D5:17:ASP:OD1   | 2.35                     | 0.60              |
| 27:DA:1018:C:O2    | 27:DA:1018:C:H2'   | 2.00                     | 0.60              |
| 27:DA:1430:C:H2'   | 27:DA:1431:U:C6    | 2.37                     | 0.60              |
| 27:DA:1775:U:C2'   | 27:DA:1776:G:H5'   | 2.25                     | 0.60              |
| 27:DA:1795:C:O2'   | 27:DA:1796:U:H5'   | 2.01                     | 0.60              |
| 25:CY:71:A:H4'     | 27:DA:1852:C:H5''  | 1.83                     | 0.60              |
| 27:DA:2362:G:H2'   | 27:DA:2363:C:H5'   | 1.82                     | 0.60              |
| 27:DA:2393:A:H5'   | 38:DP:62:LEU:HD12  | 1.83                     | 0.60              |
| 27:DA:2667:C:H2'   | 27:DA:2668:G:H5'   | 1.83                     | 0.60              |
| 27:DA:58:G:N2      | 27:DA:70:G:C4      | 2.70                     | 0.60              |
| 31:DE:93:VAL:C     | 31:DE:95:ILE:N     | 2.52                     | 0.60              |
| 32:DF:164:ARG:NH2  | 32:DF:177:ALA:HB2  | 2.17                     | 0.60              |
| 28:DB:42:C:O2      | 33:DG:93:THR:N     | 2.31                     | 0.60              |
| 35:DI:4:ILE:HD11   | 35:DI:44:LEU:CD1   | 2.31                     | 0.60              |
| 35:DI:98:ALA:HB1   | 35:DI:109:ILE:HD13 | 1.84                     | 0.60              |
| 36:DN:95:PRO:O     | 36:DN:98:VAL:HG23  | 2.01                     | 0.60              |
| 38:DP:115:LEU:HD23 | 38:DP:115:LEU:H    | 1.65                     | 0.60              |
| 38:DP:34:GLY:O     | 38:DP:35:HIS:CB    | 2.49                     | 0.60              |
| 39:DQ:58:PHE:HB3   | 39:DQ:113:GLN:HE21 | 1.66                     | 0.60              |
| 47:DY:2:ARG:N      | 47:DY:4:LYS:HG2    | 2.16                     | 0.60              |
| 1:AA:1152:A:C4     | 1:AA:1153:C:C5     | 2.90                     | 0.60              |
| 1:AA:1234:C:O2'    | 1:AA:1235:U:H5'    | 2.02                     | 0.60              |
| 1:AA:600:C:H2'     | 1:AA:601:C:C6      | 2.37                     | 0.60              |
| 3:AC:113:ALA:HB3   | 3:AC:114:PRO:CD    | 2.27                     | 0.60              |
| 5:AE:101:ILE:H     | 5:AE:101:ILE:HD13  | 1.63                     | 0.60              |
| 12:AL:15:VAL:CG2   | 12:AL:16:ARG:N     | 2.64                     | 0.60              |
| 13:AM:108:ARG:N    | 13:AM:108:ARG:HD2  | 2.17                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:2:ALA:O      | 13:AM:10:PRO:HD2   | 2.02                     | 0.60              |
| 13:AM:80:ARG:C     | 13:AM:82:MET:H     | 2.05                     | 0.60              |
| 23:AW:6:U:H2'      | 23:AW:7:A:H5''     | 1.84                     | 0.60              |
| 57:B8:32:LEU:N     | 57:B8:33:ASN:ND2   | 2.49                     | 0.60              |
| 27:BA:1181:C:O2'   | 27:BA:1182:A:H5'   | 2.01                     | 0.60              |
| 27:BA:2189:U:H5'   | 27:BA:2190:G:OP2   | 2.02                     | 0.60              |
| 27:BA:647:G:N2     | 27:BA:2350:C:O3'   | 2.35                     | 0.60              |
| 27:BA:45:C:H2'     | 27:BA:47:C:C6      | 2.37                     | 0.60              |
| 27:BA:524:U:H2'    | 27:BA:525:U:C6     | 2.37                     | 0.60              |
| 29:BC:72:VAL:HG21  | 29:BC:161:ILE:HA   | 1.84                     | 0.60              |
| 45:BW:64:MET:O     | 45:BW:65:LEU:CB    | 2.50                     | 0.60              |
| 47:BY:96:ILE:HG22  | 47:BY:97:ARG:H     | 1.64                     | 0.60              |
| 1:CA:1072:G:H2'    | 1:CA:1073:U:C6     | 2.35                     | 0.60              |
| 1:CA:1104:G:O5'    | 2:CB:111:ARG:HD2   | 2.01                     | 0.60              |
| 1:CA:1321:C:H3'    | 1:CA:1322:C:C5'    | 2.27                     | 0.60              |
| 1:CA:1255:G:H5''   | 3:CC:26:LYS:NZ     | 2.16                     | 0.60              |
| 5:CE:129:ILE:O     | 5:CE:132:ALA:N     | 2.34                     | 0.60              |
| 5:CE:69:VAL:O      | 5:CE:71:LEU:HG     | 2.02                     | 0.60              |
| 6:CF:32:ASN:C      | 6:CF:34:GLY:H      | 2.04                     | 0.60              |
| 6:CF:91:VAL:HG11   | 18:CR:72:ARG:NH1   | 2.16                     | 0.60              |
| 1:CA:1298:C:H2'    | 7:CG:114:ARG:NH1   | 2.16                     | 0.60              |
| 7:CG:11:GLN:HE22   | 7:CG:21:VAL:HG11   | 1.66                     | 0.60              |
| 8:CH:48:TYR:O      | 8:CH:49:GLU:HB3    | 2.01                     | 0.60              |
| 8:CH:63:LEU:HB2    | 8:CH:65:TYR:CE1    | 2.36                     | 0.60              |
| 14:CN:24:CYS:SG    | 14:CN:26:ARG:HG3   | 2.42                     | 0.60              |
| 19:CS:49:ILE:N     | 19:CS:49:ILE:HD12  | 2.14                     | 0.60              |
| 24:CX:19:G:H5'     | 24:CX:20:U:H5      | 1.64                     | 0.60              |
| 25:CY:54:U:H2'     | 25:CY:56:G:OP2     | 2.01                     | 0.60              |
| 27:DA:2299:G:N1    | 27:DA:2318:G:C8    | 2.70                     | 0.60              |
| 27:DA:2475:C:H5'   | 27:DA:2476:A:OP2   | 2.02                     | 0.60              |
| 27:DA:195:A:H4'    | 27:DA:251:A:O2'    | 2.02                     | 0.60              |
| 27:DA:2685:G:H5'   | 37:DO:68:GLU:OE1   | 2.02                     | 0.60              |
| 27:DA:271(Q):G:O2' | 27:DA:271(R):G:H5' | 2.02                     | 0.60              |
| 27:DA:566:U:O4     | 44:DV:78:LYS:HE2   | 2.02                     | 0.60              |
| 27:DA:802:A:C5     | 27:DA:803:U:C4     | 2.89                     | 0.60              |
| 30:DD:61:LEU:O     | 30:DD:63:ARG:NH1   | 2.34                     | 0.60              |
| 30:DD:83:GLU:HB2   | 30:DD:92:ILE:HD11  | 1.84                     | 0.60              |
| 31:DE:52:LEU:CD2   | 31:DE:76:ARG:HB2   | 2.31                     | 0.60              |
| 27:DA:2632:A:C2    | 31:DE:61:ARG:HD3   | 2.37                     | 0.60              |
| 33:DG:45:GLU:O     | 33:DG:51:ARG:HD3   | 2.02                     | 0.60              |
| 34:DH:106:THR:HG22 | 34:DH:112:PRO:HB3  | 1.84                     | 0.60              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 34:DH:26:VAL:O    | 34:DH:26:VAL:HG12   | 1.99                     | 0.60              |
| 38:DP:23:PRO:HG2  | 38:DP:33:ARG:HE     | 1.67                     | 0.60              |
| 39:DQ:56:ARG:HA   | 39:DQ:56:ARG:NH1    | 2.16                     | 0.60              |
| 39:DQ:81:VAL:HG23 | 49:D0:7:LEU:HD11    | 1.83                     | 0.60              |
| 40:DR:16:HIS:O    | 40:DR:18:LEU:N      | 2.35                     | 0.60              |
| 40:DR:66:VAL:CG1  | 40:DR:70:LEU:HD12   | 2.31                     | 0.60              |
| 46:DX:12:VAL:HG11 | 46:DX:27:THR:HG23   | 1.83                     | 0.60              |
| 1:AA:1321:C:H3'   | 1:AA:1322:C:H6      | 1.66                     | 0.60              |
| 1:AA:15:G:H4'     | 5:AE:24:ARG:NH1     | 2.13                     | 0.60              |
| 1:AA:369:C:OP2    | 1:AA:388:G:N2       | 2.34                     | 0.60              |
| 4:AD:154:ASN:C    | 4:AD:155:LEU:HD23   | 2.22                     | 0.60              |
| 1:AA:1397:C:OP2   | 5:AE:24:ARG:NH2     | 2.35                     | 0.60              |
| 10:AJ:51:ARG:HD2  | 10:AJ:59:SER:O      | 2.01                     | 0.60              |
| 13:AM:97:PRO:HA   | 13:AM:110:ARG:HD3   | 1.83                     | 0.60              |
| 15:AO:49:ASP:OD1  | 15:AO:49:ASP:C      | 2.40                     | 0.60              |
| 16:AP:20:VAL:HG23 | 16:AP:34:GLU:O      | 2.01                     | 0.60              |
| 16:AP:5:ARG:HH22  | 16:AP:26:ARG:HB2    | 1.65                     | 0.60              |
| 25:AY:14:A:N3     | 25:AY:14:A:H2'      | 2.17                     | 0.60              |
| 27:BA:2466:C:H5'' | 58:B9:6:SER:CB      | 2.32                     | 0.60              |
| 27:BA:105:C:O2'   | 47:BY:2:ARG:HB2     | 2.01                     | 0.60              |
| 27:BA:1445:A:H5'  | 27:BA:1445(A):C:OP2 | 2.01                     | 0.60              |
| 27:BA:1565:C:OP1  | 30:BD:4:LYS:NZ      | 2.34                     | 0.60              |
| 27:BA:1722:A:N6   | 27:BA:1741:A:C2     | 2.70                     | 0.60              |
| 27:BA:271(W):G:H8 | 27:BA:271(W):G:OP2  | 1.85                     | 0.60              |
| 31:BE:40:GLU:CD   | 31:BE:40:GLU:H      | 2.03                     | 0.60              |
| 31:BE:81:ILE:O    | 31:BE:82:ARG:O      | 2.19                     | 0.60              |
| 34:BH:156:ALA:HB3 | 34:BH:159:GLU:CB    | 2.32                     | 0.60              |
| 34:BH:8:PRO:HD3   | 34:BH:65:HIS:CE1    | 2.37                     | 0.60              |
| 36:BN:63:THR:H    | 36:BN:66:LYS:HD2    | 1.66                     | 0.60              |
| 42:BT:3:ARG:O     | 42:BT:4:GLY:C       | 2.40                     | 0.60              |
| 1:CA:1120:G:H2'   | 1:CA:1121:U:H6      | 1.65                     | 0.60              |
| 1:CA:428:G:O2'    | 1:CA:429:U:OP2      | 2.15                     | 0.60              |
| 2:CB:102:LEU:HD12 | 2:CB:102:LEU:N      | 2.17                     | 0.60              |
| 4:CD:104:VAL:HG21 | 4:CD:140:VAL:HG21   | 1.84                     | 0.60              |
| 4:CD:172:PRO:HD2  | 4:CD:173:TRP:CZ3    | 2.36                     | 0.60              |
| 4:CD:92:VAL:O     | 4:CD:95:GLY:N       | 2.34                     | 0.60              |
| 7:CG:65:ALA:O     | 7:CG:69:VAL:HG23    | 2.01                     | 0.60              |
| 7:CG:76:ARG:HE    | 7:CG:156:TRP:HZ2    | 1.48                     | 0.60              |
| 9:CI:52:ALA:CB    | 9:CI:95:LYS:HE2     | 2.31                     | 0.60              |
| 1:CA:1330:U:H4'   | 13:CM:23:TYR:CE2    | 2.36                     | 0.60              |
| 13:CM:69:GLU:OE1  | 13:CM:69:GLU:CA     | 2.50                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:CT:87:LYS:O     | 20:CT:91:LEU:HG    | 2.02                     | 0.60              |
| 55:D6:19:ARG:O     | 55:D6:20:ASN:O     | 2.20                     | 0.60              |
| 55:D6:39:TYR:O     | 55:D6:46:HIS:CB    | 2.45                     | 0.60              |
| 27:DA:1031:G:H4'   | 58:D9:6:SER:OG     | 2.02                     | 0.60              |
| 27:DA:2308:G:C6    | 27:DA:2310:A:H5'   | 2.36                     | 0.60              |
| 27:DA:2485:G:O2'   | 27:DA:2486:G:H5'   | 2.01                     | 0.60              |
| 27:DA:2571:C:H3'   | 27:DA:2572:A:C5'   | 2.32                     | 0.60              |
| 27:DA:851:U:H3     | 27:DA:926:A:N6     | 1.98                     | 0.60              |
| 30:DD:112:GLN:N    | 30:DD:115:GLN:NE2  | 2.49                     | 0.60              |
| 30:DD:18:VAL:CG1   | 30:DD:211:ARG:HH22 | 2.12                     | 0.60              |
| 34:DH:86:GLU:HA    | 34:DH:132:ARG:HA   | 1.84                     | 0.60              |
| 36:DN:58:ASP:O     | 36:DN:60:ILE:HG13  | 2.02                     | 0.60              |
| 38:DP:130:PHE:N    | 38:DP:130:PHE:CD2  | 2.69                     | 0.60              |
| 42:DT:8:LYS:HA     | 42:DT:11:GLU:OE2   | 2.00                     | 0.60              |
| 46:DX:35:THR:HG22  | 46:DX:37:THR:N     | 2.17                     | 0.60              |
| 39:DQ:134:ARG:HH21 | 48:DZ:121:ARG:NH1  | 2.00                     | 0.60              |
| 48:DZ:56:ILE:HG22  | 48:DZ:57:VAL:H     | 1.67                     | 0.60              |
| 1:AA:324:G:H8      | 1:AA:324:G:H3'     | 1.67                     | 0.60              |
| 1:AA:407:G:N2      | 1:AA:436:C:C2      | 2.70                     | 0.60              |
| 1:AA:911:U:H2'     | 1:AA:912:C:C5      | 2.36                     | 0.60              |
| 2:AB:215:LEU:O     | 2:AB:219:VAL:HG23  | 2.02                     | 0.60              |
| 3:AC:186:PHE:CE2   | 3:AC:188:LEU:HD22  | 2.36                     | 0.60              |
| 4:AD:98:GLU:O      | 4:AD:100:ARG:N     | 2.35                     | 0.60              |
| 5:AE:100:VAL:HG22  | 5:AE:118:ILE:HG22  | 1.83                     | 0.60              |
| 7:AG:15:ASP:OD2    | 7:AG:44:TYR:OH     | 2.20                     | 0.60              |
| 8:AH:2:LEU:HD13    | 8:AH:2:LEU:C       | 2.23                     | 0.60              |
| 15:AO:82:ILE:HD13  | 15:AO:82:ILE:C     | 2.23                     | 0.60              |
| 16:AP:67:THR:HB    | 16:AP:70:ALA:HB2   | 1.84                     | 0.60              |
| 19:AS:29:ARG:HD2   | 19:AS:30:LEU:N     | 2.17                     | 0.60              |
| 20:AT:97:ALA:O     | 20:AT:99:LEU:N     | 2.34                     | 0.60              |
| 50:B1:19:GLN:O     | 50:B1:35:THR:N     | 2.34                     | 0.60              |
| 27:BA:2231:C:OP1   | 50:B1:42:GLN:HA    | 2.01                     | 0.60              |
| 54:B5:56:LYS:HG3   | 54:B5:59:GLU:CG    | 2.32                     | 0.60              |
| 27:BA:2350:C:H5''  | 57:B8:42:ARG:HD3   | 1.84                     | 0.60              |
| 27:BA:1891:G:H2'   | 27:BA:1892:C:C6    | 2.37                     | 0.60              |
| 27:BA:2084:C:H2'   | 27:BA:2085:C:H6    | 1.67                     | 0.60              |
| 27:BA:557:U:H2'    | 27:BA:558:G:H8     | 1.67                     | 0.60              |
| 27:BA:875:G:H2'    | 27:BA:876:C:O4'    | 2.01                     | 0.60              |
| 30:BD:70:TRP:CZ3   | 30:BD:146:GLU:CD   | 2.75                     | 0.60              |
| 32:BF:126:VAL:HG23 | 32:BF:127:GLU:N    | 2.16                     | 0.60              |
| 32:BF:9:ILE:HG12   | 32:BF:14:PRO:HA    | 1.83                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:BH:125:VAL:HG12 | 34:BH:125:VAL:O   | 2.01                     | 0.60              |
| 34:BH:109:PHE:CE1  | 34:BH:152:ARG:CZ  | 2.85                     | 0.60              |
| 36:BN:132:ALA:O    | 36:BN:133:GLN:HB3 | 2.02                     | 0.60              |
| 38:BP:47:ASP:OD1   | 38:BP:49:ARG:HB2  | 2.01                     | 0.60              |
| 42:BT:16:ARG:HH12  | 42:BT:19:LEU:HD21 | 1.67                     | 0.60              |
| 46:BX:12:VAL:CG2   | 46:BX:13:LEU:H    | 2.01                     | 0.60              |
| 1:CA:1079:G:H2'    | 1:CA:1080:A:C8    | 2.36                     | 0.60              |
| 1:CA:1326:C:OP1    | 21:CU:12:LYS:HD2  | 2.02                     | 0.60              |
| 1:CA:653:A:C1'     | 8:CH:56:LYS:HZ3   | 2.15                     | 0.60              |
| 2:CB:198:ASP:N     | 2:CB:198:ASP:OD2  | 2.34                     | 0.60              |
| 2:CB:204:ASN:HD21  | 2:CB:207:ALA:CB   | 2.03                     | 0.60              |
| 9:CI:106:ALA:O     | 9:CI:108:VAL:HG13 | 2.02                     | 0.60              |
| 12:CL:82:ILE:CG2   | 12:CL:95:TYR:HD2  | 2.15                     | 0.60              |
| 15:CO:35:ARG:HH21  | 15:CO:59:MET:CE   | 2.06                     | 0.60              |
| 18:CR:50:ILE:HD11  | 18:CR:70:ILE:HG21 | 1.84                     | 0.60              |
| 23:CW:20:A:H62     | 23:CW:44:A:C2'    | 2.12                     | 0.60              |
| 25:CY:52:G:H2'     | 25:CY:53:U:C6     | 2.37                     | 0.60              |
| 27:DA:1122:G:O2'   | 27:DA:1123:C:H5'  | 2.02                     | 0.60              |
| 27:DA:1569:A:H1'   | 30:DD:38:LYS:HZ3  | 1.65                     | 0.60              |
| 27:DA:2236:C:H2'   | 27:DA:2237:G:O4'  | 2.02                     | 0.60              |
| 27:DA:2593:U:H2'   | 27:DA:2594:C:H6   | 1.65                     | 0.60              |
| 27:DA:2684:U:H2'   | 27:DA:2685:G:O4'  | 2.01                     | 0.60              |
| 32:DF:123:LEU:HA   | 32:DF:192:LEU:O   | 2.02                     | 0.60              |
| 32:DF:195:ASP:OD2  | 32:DF:195:ASP:N   | 2.34                     | 0.60              |
| 36:DN:103:VAL:O    | 36:DN:107:LEU:HG  | 2.02                     | 0.60              |
| 38:DP:23:PRO:HD2   | 38:DP:33:ARG:HH21 | 1.67                     | 0.60              |
| 40:DR:12:ARG:HD3   | 40:DR:16:HIS:ND1  | 2.17                     | 0.60              |
| 42:DT:11:GLU:O     | 42:DT:13:ARG:N    | 2.25                     | 0.60              |
| 44:DV:38:LEU:O     | 44:DV:52:VAL:HG12 | 2.01                     | 0.60              |
| 45:DW:13:SER:O     | 45:DW:16:LYS:HB2  | 2.01                     | 0.60              |
| 48:DZ:97:MET:O     | 48:DZ:124:LEU:HA  | 2.02                     | 0.60              |
| 48:DZ:157:PRO:HB2  | 48:DZ:158:PRO:HD2 | 1.83                     | 0.60              |
| 1:AA:1146:A:H2'    | 1:AA:1147:C:H5''  | 1.83                     | 0.59              |
| 1:AA:1366:C:H2'    | 1:AA:1367:C:C6    | 2.33                     | 0.59              |
| 1:AA:399:G:H2'     | 1:AA:400:C:C6     | 2.37                     | 0.59              |
| 4:AD:17:VAL:HG11   | 4:AD:197:PRO:CG   | 2.27                     | 0.59              |
| 6:AF:75:LEU:CD2    | 6:AF:79:LEU:HG    | 2.32                     | 0.59              |
| 7:AG:41:ARG:O      | 7:AG:45:ASP:HB2   | 2.02                     | 0.59              |
| 8:AH:87:SER:HB2    | 8:AH:93:VAL:HB    | 1.84                     | 0.59              |
| 13:AM:69:GLU:OE1   | 13:AM:72:ALA:HB3  | 2.01                     | 0.59              |
| 24:AX:24:U:O2'     | 27:BA:1923:U:OP1  | 2.19                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AX:6:G:H2'      | 24:AX:7:G:O4'      | 2.02                     | 0.59              |
| 54:B5:6:VAL:HG22   | 54:B5:7:PRO:HD2    | 1.84                     | 0.59              |
| 27:BA:2068:U:N3    | 27:BA:2430:A:H2    | 1.86                     | 0.59              |
| 32:BF:135:LYS:HB3  | 32:BF:138:GLU:CD   | 2.22                     | 0.59              |
| 33:BG:107:LEU:HD22 | 33:BG:177:GLY:O    | 2.01                     | 0.59              |
| 37:BO:10:VAL:HG21  | 37:BO:17:ARG:HA    | 1.84                     | 0.59              |
| 42:BT:16:ARG:NH1   | 42:BT:19:LEU:HD21  | 2.17                     | 0.59              |
| 43:BU:34:LYS:CE    | 43:BU:34:LYS:HA    | 2.30                     | 0.59              |
| 43:BU:42:ALA:O     | 43:BU:45:TYR:N     | 2.35                     | 0.59              |
| 1:CA:1168:A:H3'    | 1:CA:1169:A:H8     | 1.65                     | 0.59              |
| 1:CA:1346:A:N7     | 7:CG:10:ARG:NH2    | 2.50                     | 0.59              |
| 1:CA:620:C:H2'     | 1:CA:621:A:O4'     | 2.02                     | 0.59              |
| 2:CB:81:VAL:HB     | 2:CB:94:ASN:OD1    | 2.02                     | 0.59              |
| 3:CC:35:GLU:HA     | 3:CC:38:ARG:HD2    | 1.84                     | 0.59              |
| 7:CG:65:ALA:HB3    | 7:CG:124:LEU:HD23  | 1.82                     | 0.59              |
| 8:CH:28:ALA:HA     | 8:CH:59:LEU:CD1    | 2.32                     | 0.59              |
| 11:CK:93:GLN:OE1   | 11:CK:93:GLN:HA    | 2.01                     | 0.59              |
| 19:CS:24:ALA:O     | 19:CS:25:LYS:HB2   | 2.02                     | 0.59              |
| 25:CY:37:U:C2'     | 25:CY:38:U:H5''    | 2.32                     | 0.59              |
| 49:D0:20:ARG:HG2   | 49:D0:20:ARG:HH11  | 1.66                     | 0.59              |
| 27:DA:2527:C:H5'   | 58:D9:30:PRO:CB    | 2.31                     | 0.59              |
| 27:DA:1490:A:H5'   | 27:DA:1494:A:N6    | 2.17                     | 0.59              |
| 27:DA:172:C:O2'    | 27:DA:173:G:H8     | 1.84                     | 0.59              |
| 27:DA:2298:A:H2'   | 27:DA:2299:G:H8    | 1.65                     | 0.59              |
| 27:DA:2498:C:HO2'  | 27:DA:2499:C:H5''  | 1.66                     | 0.59              |
| 27:DA:2531:A:N6    | 27:DA:2662:A:H61   | 2.00                     | 0.59              |
| 27:DA:2748:A:N7    | 27:DA:2754:U:O4    | 2.35                     | 0.59              |
| 27:DA:94(A):G:C3'  | 27:DA:95:G:H5''    | 2.32                     | 0.59              |
| 27:DA:962:G:H2'    | 27:DA:963:U:O4'    | 2.02                     | 0.59              |
| 27:DA:1829:A:N3    | 30:DD:15:PHE:HZ    | 2.00                     | 0.59              |
| 31:DE:14:ILE:HB    | 42:DT:14:TYR:CE2   | 2.37                     | 0.59              |
| 31:DE:37:ARG:HB2   | 31:DE:46:ALA:H     | 1.66                     | 0.59              |
| 32:DF:83:PHE:O     | 32:DF:84:VAL:HB    | 2.02                     | 0.59              |
| 33:DG:41:GLN:HE22  | 33:DG:153:ARG:CG   | 2.15                     | 0.59              |
| 34:DH:89:ILE:HG22  | 34:DH:162:ILE:HG23 | 1.84                     | 0.59              |
| 40:DR:44:LEU:HD13  | 40:DR:44:LEU:O     | 2.02                     | 0.59              |
| 42:DT:26:ASP:HB3   | 42:DT:89:VAL:O     | 2.02                     | 0.59              |
| 46:DX:81:VAL:O     | 46:DX:81:VAL:HG23  | 2.02                     | 0.59              |
| 1:AA:1028:C:H2'    | 1:AA:1029:C:H5'    | 1.83                     | 0.59              |
| 1:AA:1238:A:H2     | 1:AA:1241:G:H1'    | 1.66                     | 0.59              |
| 1:AA:1288:A:O2'    | 1:AA:1289:A:H5'    | 2.02                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1349:A:OP1   | 9:AI:121:ARG:N     | 2.31                     | 0.59              |
| 1:AA:389:A:H2'    | 1:AA:390:C:C5'     | 2.32                     | 0.59              |
| 1:AA:577:G:H4'    | 1:AA:816:A:O2'     | 2.02                     | 0.59              |
| 1:AA:621:A:H2'    | 1:AA:622:A:C8      | 2.37                     | 0.59              |
| 1:AA:782:A:C2     | 1:AA:801:U:C2      | 2.90                     | 0.59              |
| 1:AA:986:A:O2'    | 1:AA:987:G:H5'     | 2.01                     | 0.59              |
| 6:AF:100:ASN:HD21 | 18:AR:23:LYS:HG2   | 1.66                     | 0.59              |
| 15:AO:33:THR:HG22 | 15:AO:33:THR:O     | 2.02                     | 0.59              |
| 18:AR:53:ARG:CZ   | 18:AR:60:ALA:H     | 2.15                     | 0.59              |
| 20:AT:33:ILE:CD1  | 20:AT:63:ILE:HA    | 2.32                     | 0.59              |
| 7:AG:148:ASN:HD21 | 25:AY:39:C:H4'     | 1.66                     | 0.59              |
| 53:B4:60:GLU:O    | 53:B4:61:VAL:CB    | 2.50                     | 0.59              |
| 57:B8:29:LYS:HG3  | 57:B8:29:LYS:O     | 2.02                     | 0.59              |
| 27:BA:2400:G:H5'  | 27:BA:2401:U:OP2   | 2.02                     | 0.59              |
| 27:BA:2466:C:C2'  | 27:BA:2467:C:H5'   | 2.32                     | 0.59              |
| 27:BA:2547:U:H2'  | 27:BA:2548:G:C8    | 2.37                     | 0.59              |
| 27:BA:2589:A:O2'  | 27:BA:2590:A:H5'   | 2.02                     | 0.59              |
| 27:BA:2636:U:O2'  | 31:BE:44:TYR:CE1   | 2.55                     | 0.59              |
| 27:BA:2670:A:C2'  | 27:BA:2671:A:H5'   | 2.32                     | 0.59              |
| 27:BA:971:C:C2'   | 27:BA:972:G:H5'    | 2.32                     | 0.59              |
| 28:BB:42:C:O2     | 33:BG:93:THR:N     | 2.34                     | 0.59              |
| 28:BB:8:U:C5'     | 28:BB:8:U:H6       | 2.14                     | 0.59              |
| 30:BD:30:GLU:CD   | 30:BD:63:ARG:NH2   | 2.55                     | 0.59              |
| 27:BA:779:U:P     | 30:BD:49:ILE:HG22  | 2.43                     | 0.59              |
| 35:BI:136:VAL:O   | 35:BI:136:VAL:HG13 | 2.02                     | 0.59              |
| 38:BP:84:ASN:ND2  | 38:BP:115:LEU:CG   | 2.65                     | 0.59              |
| 48:BZ:152:SER:H   | 48:BZ:166:PRO:CB   | 2.14                     | 0.59              |
| 1:CA:1177:G:N1    | 1:CA:1181:G:C6     | 2.70                     | 0.59              |
| 1:CA:1368:G:N2    | 1:CA:1369:C:H1'    | 2.17                     | 0.59              |
| 1:CA:320:C:H1'    | 1:CA:1434:A:C2     | 2.35                     | 0.59              |
| 1:CA:752:G:H1'    | 1:CA:754:C:N4      | 2.18                     | 0.59              |
| 1:CA:943:U:H6     | 1:CA:943:U:O5'     | 1.84                     | 0.59              |
| 9:CI:40:LEU:C     | 9:CI:42:ARG:H      | 2.05                     | 0.59              |
| 24:CX:17:C:C3'    | 24:CX:17(B):U:H5'  | 2.31                     | 0.59              |
| 56:D7:24:THR:HG23 | 56:D7:27:GLY:CA    | 2.32                     | 0.59              |
| 27:DA:1482:G:N2   | 27:DA:1507:A:H1'   | 2.16                     | 0.59              |
| 27:DA:1830:C:H42  | 27:DA:1975:G:H1    | 1.50                     | 0.59              |
| 27:DA:2576:G:H5'' | 27:DA:2577:A:OP1   | 2.02                     | 0.59              |
| 27:DA:2611:U:H1'  | 54:D5:3:LYS:CE     | 2.30                     | 0.59              |
| 30:DD:27:THR:HG23 | 30:DD:27:THR:O     | 2.01                     | 0.59              |
| 30:DD:66:ASP:HB3  | 30:DD:105:ILE:HD13 | 1.84                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DD:93:ALA:HB2   | 30:DD:107:ALA:HB2  | 1.83                     | 0.59              |
| 34:DH:70:THR:O     | 34:DH:72:ILE:N     | 2.35                     | 0.59              |
| 35:DI:94:ALA:HB1   | 35:DI:114:LEU:HD11 | 1.84                     | 0.59              |
| 37:DO:36:GLY:O     | 37:DO:109:LYS:HG3  | 2.01                     | 0.59              |
| 42:DT:48:ILE:HG22  | 42:DT:50:ILE:HD12  | 1.84                     | 0.59              |
| 42:DT:61:PHE:CE2   | 42:DT:76:PHE:HB2   | 2.37                     | 0.59              |
| 43:DU:20:LEU:O     | 43:DU:20:LEU:HD13  | 2.02                     | 0.59              |
| 27:DA:2012:G:O3'   | 45:DW:96:ILE:HD11  | 2.02                     | 0.59              |
| 27:DA:328:U:H4'    | 47:DY:68:HIS:CE1   | 2.36                     | 0.59              |
| 1:AA:578:C:HO2'    | 1:AA:579:G:H8      | 1.50                     | 0.59              |
| 3:AC:90:GLU:OE1    | 3:AC:93:LYS:HD2    | 2.03                     | 0.59              |
| 4:AD:59:ARG:HH21   | 4:AD:66:ARG:NH2    | 2.00                     | 0.59              |
| 6:AF:6:VAL:HG13    | 6:AF:90:VAL:HG22   | 1.84                     | 0.59              |
| 7:AG:15:ASP:H      | 7:AG:20:ASP:N      | 2.00                     | 0.59              |
| 8:AH:80:ILE:HG22   | 8:AH:80:ILE:O      | 2.02                     | 0.59              |
| 9:AI:48:GLU:O      | 9:AI:50:LEU:N      | 2.36                     | 0.59              |
| 17:AQ:45:HIS:HA    | 17:AQ:69:LYS:NZ    | 2.17                     | 0.59              |
| 51:B2:41:ILE:HD11  | 51:B2:44:LEU:CB    | 2.31                     | 0.59              |
| 52:B3:43:ILE:O     | 52:B3:47:VAL:HG23  | 2.01                     | 0.59              |
| 56:B7:5:TRP:HH2    | 56:B7:12:ARG:HH12  | 1.50                     | 0.59              |
| 27:BA:592:G:N2     | 27:BA:666:G:C4     | 2.70                     | 0.59              |
| 27:BA:782:A:O5'    | 27:BA:783:A:N1     | 2.35                     | 0.59              |
| 31:BE:184:VAL:HG12 | 31:BE:185:LYS:H    | 1.66                     | 0.59              |
| 31:BE:55:ASN:O     | 31:BE:57:LYS:N     | 2.33                     | 0.59              |
| 36:BN:46:VAL:HG13  | 36:BN:47:ALA:N     | 2.18                     | 0.59              |
| 42:BT:68:TYR:O     | 42:BT:69:GLY:C     | 2.40                     | 0.59              |
| 1:CA:1073:U:H2'    | 1:CA:1074:G:C8     | 2.35                     | 0.59              |
| 1:CA:1170:A:H2'    | 1:CA:1171:G:H5'    | 1.84                     | 0.59              |
| 1:CA:1186:G:N2     | 1:CA:1187:G:H1'    | 2.17                     | 0.59              |
| 1:CA:384:G:H2'     | 1:CA:385:C:C6      | 2.37                     | 0.59              |
| 9:CI:17:VAL:HG21   | 9:CI:80:GLY:HA3    | 1.83                     | 0.59              |
| 12:CL:100:GLY:HA2  | 12:CL:104:ALA:O    | 2.02                     | 0.59              |
| 12:CL:21:VAL:CG1   | 12:CL:21:VAL:O     | 2.49                     | 0.59              |
| 13:CM:31:LYS:HA    | 13:CM:34:LEU:CG    | 2.32                     | 0.59              |
| 14:CN:39:LEU:CD1   | 14:CN:44:LEU:HA    | 2.31                     | 0.59              |
| 16:CP:20:VAL:HG22  | 16:CP:21:VAL:N     | 2.18                     | 0.59              |
| 17:CQ:62:SER:CB    | 17:CQ:72:ARG:HG3   | 2.32                     | 0.59              |
| 20:CT:41:ILE:HG13  | 20:CT:41:ILE:O     | 2.01                     | 0.59              |
| 50:D1:44:PRO:HB2   | 50:D1:46:LEU:HD13  | 1.83                     | 0.59              |
| 27:DA:2015:A:H1'   | 54:D5:2:ALA:HA     | 1.84                     | 0.59              |
| 27:DA:1341:U:H2'   | 27:DA:1397:U:O2'   | 2.02                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:1678:G:N2    | 27:DA:1989:G:H1   | 2.01                     | 0.59              |
| 27:DA:1771:C:H1'   | 27:DA:1786:A:C8   | 2.37                     | 0.59              |
| 27:DA:2053:G:O2'   | 27:DA:2054:A:H5'  | 2.01                     | 0.59              |
| 27:DA:2069:G:C2    | 27:DA:2070:G:C8   | 2.89                     | 0.59              |
| 27:DA:221:A:H8     | 27:DA:221:A:OP2   | 1.85                     | 0.59              |
| 27:DA:2579:C:H2'   | 27:DA:2580:U:H6   | 1.67                     | 0.59              |
| 27:DA:2663:G:O2'   | 27:DA:2664:G:H5'  | 2.02                     | 0.59              |
| 27:DA:827:U:H4'    | 27:DA:828:U:O2    | 2.02                     | 0.59              |
| 27:DA:857:C:OP2    | 49:D0:77:ARG:NH2  | 2.35                     | 0.59              |
| 27:DA:2073:C:O3'   | 30:DD:228:PRO:HB3 | 2.02                     | 0.59              |
| 30:DD:83:GLU:O     | 30:DD:92:ILE:HD13 | 2.03                     | 0.59              |
| 34:DH:85:LYS:HD3   | 34:DH:133:VAL:HB  | 1.85                     | 0.59              |
| 39:DQ:110:THR:HG23 | 39:DQ:113:GLN:HB2 | 1.84                     | 0.59              |
| 44:DV:75:PHE:CD2   | 44:DV:82:ARG:HG3  | 2.37                     | 0.59              |
| 46:DX:64:LYS:NZ    | 46:DX:73:ARG:NH2  | 2.50                     | 0.59              |
| 48:DZ:58:LEU:O     | 48:DZ:65:SER:HA   | 2.01                     | 0.59              |
| 1:AA:163:C:H2'     | 1:AA:164:U:H6     | 1.67                     | 0.59              |
| 1:AA:189(K):U:H2'  | 1:AA:189(L):G:H8  | 1.64                     | 0.59              |
| 1:AA:495:A:C1'     | 1:AA:496:A:H5'    | 2.32                     | 0.59              |
| 1:AA:606:G:H2'     | 1:AA:631:G:N1     | 2.16                     | 0.59              |
| 1:AA:920:U:H5'     | 1:AA:921:U:OP2    | 2.02                     | 0.59              |
| 3:AC:113:ALA:CB    | 3:AC:114:PRO:HD3  | 2.30                     | 0.59              |
| 4:AD:30:LYS:C      | 4:AD:32:ALA:H     | 2.02                     | 0.59              |
| 27:BA:1175:U:H4'   | 27:BA:1176:G:H3'  | 1.83                     | 0.59              |
| 27:BA:1417:C:N4    | 27:BA:1581:G:H1   | 2.00                     | 0.59              |
| 27:BA:1710:C:H3'   | 27:BA:1710:C:H6   | 1.66                     | 0.59              |
| 27:BA:1762:A:H8    | 27:BA:1762:A:O5'  | 1.84                     | 0.59              |
| 27:BA:258:G:H2'    | 27:BA:259:G:H8    | 1.66                     | 0.59              |
| 1:AA:1442(A):G:N1  | 27:BA:2864:G:OP1  | 2.33                     | 0.59              |
| 27:BA:347:A:H2'    | 27:BA:348:G:C8    | 2.37                     | 0.59              |
| 27:BA:70:G:O2'     | 27:BA:114:U:H5    | 1.85                     | 0.59              |
| 27:BA:841:A:H2'    | 27:BA:842:G:H8    | 1.67                     | 0.59              |
| 27:BA:875:G:O2'    | 27:BA:876:C:H5'   | 2.02                     | 0.59              |
| 32:BF:25:PRO:HG3   | 32:BF:119:ARG:HA  | 1.85                     | 0.59              |
| 35:BI:145:VAL:HG12 | 35:BI:146:ALA:N   | 2.18                     | 0.59              |
| 35:BI:23:PRO:O     | 35:BI:26:ALA:HB3  | 2.02                     | 0.59              |
| 40:BR:20:LEU:CD1   | 40:BR:24:GLN:HG3  | 2.32                     | 0.59              |
| 41:BS:17:ARG:O     | 41:BS:18:ILE:HB   | 2.02                     | 0.59              |
| 41:BS:93:LYS:O     | 41:BS:94:TYR:C    | 2.40                     | 0.59              |
| 47:BY:46:LYS:C     | 47:BY:47:LYS:HG3  | 2.21                     | 0.59              |
| 1:CA:1137:C:C4'    | 1:CA:1138:G:C2    | 2.79                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:14:U:H5'     | 1:CA:14:U:C6       | 2.37                     | 0.59              |
| 1:CA:392:G:H2'    | 1:CA:393:A:C8      | 2.37                     | 0.59              |
| 1:CA:821:G:H2'    | 1:CA:822:C:C6      | 2.34                     | 0.59              |
| 2:CB:200:ILE:CG2  | 2:CB:201:ILE:N     | 2.65                     | 0.59              |
| 5:CE:141:GLN:HA   | 5:CE:143:ARG:NH2   | 2.18                     | 0.59              |
| 5:CE:7:GLU:O      | 5:CE:8:GLU:HB3     | 2.03                     | 0.59              |
| 9:CI:52:ALA:HB3   | 9:CI:95:LYS:HE2    | 1.83                     | 0.59              |
| 18:CR:64:ARG:O    | 18:CR:67:ALA:N     | 2.35                     | 0.59              |
| 19:CS:58:VAL:HG23 | 19:CS:58:VAL:O     | 2.01                     | 0.59              |
| 27:DA:1014:U:H2'  | 27:DA:1015:G:H8    | 1.66                     | 0.59              |
| 27:DA:173:G:H2'   | 27:DA:174:C:C6     | 2.37                     | 0.59              |
| 27:DA:2498:C:O2'  | 27:DA:2499:C:C5'   | 2.45                     | 0.59              |
| 27:DA:363:G:H2'   | 27:DA:363(A):A:C8  | 2.38                     | 0.59              |
| 27:DA:630:G:N1    | 27:DA:634:C:N4     | 2.47                     | 0.59              |
| 27:DA:651:G:H2'   | 27:DA:651:G:N3     | 2.17                     | 0.59              |
| 27:DA:660:G:C2    | 27:DA:661:C:H1'    | 2.38                     | 0.59              |
| 27:DA:947:G:N2    | 27:DA:971:C:C2     | 2.70                     | 0.59              |
| 29:DC:24:GLU:HB3  | 29:DC:27:ARG:NH2   | 2.18                     | 0.59              |
| 30:DD:60:ARG:CG   | 30:DD:86:PRO:HB3   | 2.30                     | 0.59              |
| 33:DG:119:GLY:O   | 33:DG:181:ARG:HB2  | 2.02                     | 0.59              |
| 33:DG:31:VAL:HG22 | 33:DG:32:PRO:HD2   | 1.85                     | 0.59              |
| 34:DH:38:SER:O    | 34:DH:40:GLU:N     | 2.34                     | 0.59              |
| 27:DA:2749:A:H1'  | 34:DH:63:SER:OG    | 2.02                     | 0.59              |
| 36:DN:99:LEU:O    | 36:DN:103:VAL:HG23 | 2.03                     | 0.59              |
| 36:DN:41:ASP:O    | 36:DN:42:TRP:O     | 2.21                     | 0.59              |
| 36:DN:57:ALA:O    | 36:DN:58:ASP:C     | 2.40                     | 0.59              |
| 38:DP:107:LYS:O   | 38:DP:109:GLY:N    | 2.36                     | 0.59              |
| 41:DS:17:ARG:HA   | 41:DS:20:ARG:NE    | 2.17                     | 0.59              |
| 47:DY:28:LYS:HB2  | 47:DY:37:VAL:HB    | 1.84                     | 0.59              |
| 47:DY:42:VAL:CB   | 47:DY:65:ALA:HB3   | 2.23                     | 0.59              |
| 1:AA:1323:G:H2'   | 1:AA:1324:A:C8     | 2.38                     | 0.59              |
| 1:AA:1417:G:H22   | 1:AA:1482:G:H2'    | 1.67                     | 0.59              |
| 1:AA:818:G:C2'    | 1:AA:819:A:H5''    | 2.32                     | 0.59              |
| 1:AA:936:C:H2'    | 1:AA:937:A:O4'     | 2.01                     | 0.59              |
| 3:AC:73:PRO:C     | 3:AC:75:VAL:H      | 2.06                     | 0.59              |
| 4:AD:196:LEU:N    | 4:AD:196:LEU:CD1   | 2.61                     | 0.59              |
| 1:AA:1152:A:OP1   | 10:AJ:68:HIS:CD2   | 2.56                     | 0.59              |
| 51:B2:13:ALA:HA   | 51:B2:16:LEU:HD11  | 1.83                     | 0.59              |
| 53:B4:39:ARG:C    | 53:B4:40:ILE:HD12  | 2.23                     | 0.59              |
| 55:B6:27:LYS:HB3  | 55:B6:29:ASN:OD1   | 2.02                     | 0.59              |
| 27:BA:1997:G:O2'  | 27:BA:1998:G:H5'   | 2.02                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:2585:U:H4'   | 27:BA:2586:C:O5'  | 2.01                     | 0.59              |
| 27:BA:479:A:H4'    | 27:BA:480:A:OP1   | 2.02                     | 0.59              |
| 27:BA:592:G:H1     | 27:BA:665:C:N4    | 1.99                     | 0.59              |
| 32:BF:9:ILE:HG23   | 32:BF:13:SER:O    | 2.01                     | 0.59              |
| 37:BO:117:LEU:HD23 | 37:BO:117:LEU:O   | 2.02                     | 0.59              |
| 37:BO:59:LYS:CD    | 37:BO:89:ASN:OD1  | 2.50                     | 0.59              |
| 38:BP:41:ARG:HG2   | 38:BP:41:ARG:HH21 | 1.65                     | 0.59              |
| 43:BU:95:LEU:HD21  | 44:BV:13:ARG:HB2  | 1.83                     | 0.59              |
| 48:BZ:130:ARG:HH11 | 48:BZ:130:ARG:HG2 | 1.68                     | 0.59              |
| 1:CA:107:G:O2'     | 1:CA:108:G:H5'    | 2.02                     | 0.59              |
| 1:CA:489:C:O2'     | 1:CA:490:G:H5'    | 2.02                     | 0.59              |
| 1:CA:503:C:OP2     | 12:CL:113:SER:OG  | 2.16                     | 0.59              |
| 1:CA:965:A:C4'     | 1:CA:966:G:OP1    | 2.50                     | 0.59              |
| 1:CA:965:A:C2      | 1:CA:969:A:C2     | 2.91                     | 0.59              |
| 16:CP:20:VAL:HG21  | 16:CP:32:TYR:CG   | 2.37                     | 0.59              |
| 17:CQ:64:PRO:HA    | 17:CQ:70:ARG:HG2  | 1.83                     | 0.59              |
| 27:DA:2884:U:OP2   | 54:D5:43:HIS:CE1  | 2.55                     | 0.59              |
| 55:D6:19:ARG:CG    | 55:D6:20:ASN:H    | 2.15                     | 0.59              |
| 27:DA:1349:A:N6    | 27:DA:1598:C:N4   | 2.51                     | 0.59              |
| 27:DA:1655:A:C4'   | 31:DE:114:ALA:HA  | 2.31                     | 0.59              |
| 27:DA:1702:G:C2'   | 27:DA:1703:G:O5'  | 2.51                     | 0.59              |
| 27:DA:200:U:H6     | 27:DA:200:U:C5'   | 2.08                     | 0.59              |
| 27:DA:2443:C:H2'   | 27:DA:2444:G:C8   | 2.32                     | 0.59              |
| 27:DA:2469:A:N6    | 27:DA:2481:G:H1'  | 2.18                     | 0.59              |
| 27:DA:2826:A:N3    | 27:DA:2826:A:H2'  | 2.16                     | 0.59              |
| 27:DA:357:A:H2'    | 27:DA:358:U:C6    | 2.38                     | 0.59              |
| 27:DA:662:G:H2'    | 27:DA:663:G:C8    | 2.36                     | 0.59              |
| 27:DA:896:A:C2     | 48:DZ:113:GLY:HA3 | 2.38                     | 0.59              |
| 29:DC:20:TYR:CE1   | 29:DC:22:ILE:HD13 | 2.37                     | 0.59              |
| 30:DD:142:VAL:HG23 | 30:DD:192:THR:O   | 2.01                     | 0.59              |
| 32:DF:3:GLU:HB3    | 32:DF:20:LEU:O    | 2.01                     | 0.59              |
| 33:DG:60:LEU:HD13  | 33:DG:60:LEU:C    | 2.23                     | 0.59              |
| 33:DG:46:ALA:C     | 33:DG:82:LEU:HD11 | 2.23                     | 0.59              |
| 34:DH:85:LYS:HG2   | 34:DH:133:VAL:HB  | 1.84                     | 0.59              |
| 35:DI:79:ILE:HG22  | 35:DI:81:VAL:HG22 | 1.83                     | 0.59              |
| 27:DA:558:G:P      | 36:DN:111:PRO:HD2 | 2.42                     | 0.59              |
| 44:DV:32:THR:HG22  | 44:DV:32:THR:O    | 2.03                     | 0.59              |
| 46:DX:31:HIS:ND1   | 46:DX:32:PRO:HD2  | 2.18                     | 0.59              |
| 1:AA:115:G:O2'     | 1:AA:116:A:OP2    | 2.19                     | 0.59              |
| 1:AA:1228:C:O3'    | 13:AM:116:THR:HA  | 2.03                     | 0.59              |
| 1:AA:299:G:H2'     | 1:AA:300:A:H8     | 1.64                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:479:C:H2'     | 1:AA:480:U:C6      | 2.38                     | 0.59              |
| 1:AA:583:A:H61     | 1:AA:758:G:H1'     | 1.67                     | 0.59              |
| 1:AA:910:C:O2'     | 1:AA:911:U:H5'     | 2.03                     | 0.59              |
| 1:AA:929:G:O2'     | 1:AA:930:C:H5'     | 2.03                     | 0.59              |
| 1:AA:939:G:C5'     | 7:AG:102:ARG:HH12  | 2.16                     | 0.59              |
| 5:AE:139:LEU:HA    | 5:AE:142:LEU:CD1   | 2.32                     | 0.59              |
| 6:AF:80:ARG:C      | 6:AF:82:ARG:H      | 2.05                     | 0.59              |
| 8:AH:100:ILE:HB    | 8:AH:125:ARG:HH12  | 1.67                     | 0.59              |
| 10:AJ:4:ILE:HG12   | 10:AJ:100:THR:HG21 | 1.84                     | 0.59              |
| 12:AL:31:ARG:HG2   | 12:AL:32:GLY:N     | 2.17                     | 0.59              |
| 27:BA:1387:C:O5'   | 27:BA:1387:C:H6    | 1.85                     | 0.59              |
| 27:BA:1594:G:H3'   | 27:BA:1595:G:H8    | 1.68                     | 0.59              |
| 27:BA:1754:C:C6    | 42:BT:96:ARG:NH1   | 2.70                     | 0.59              |
| 27:BA:2068:U:H5''  | 27:BA:2068:U:H6    | 1.67                     | 0.59              |
| 27:BA:2350:C:C5'   | 57:B8:42:ARG:HD3   | 2.32                     | 0.59              |
| 27:BA:2384:G:H2'   | 27:BA:2386:C:OP1   | 2.03                     | 0.59              |
| 30:BD:35:LYS:HZ3   | 30:BD:102:LYS:C    | 2.05                     | 0.59              |
| 32:BF:40:GLN:O     | 32:BF:44:ARG:HG2   | 2.02                     | 0.59              |
| 36:BN:121:LYS:HB3  | 36:BN:123:TYR:HE1  | 1.67                     | 0.59              |
| 36:BN:58:ASP:C     | 36:BN:60:ILE:H     | 2.03                     | 0.59              |
| 42:BT:47:GLY:HA3   | 42:BT:64:ARG:O     | 2.01                     | 0.59              |
| 42:BT:68:TYR:N     | 42:BT:68:TYR:CD2   | 2.69                     | 0.59              |
| 42:BT:91:ARG:HA    | 42:BT:117:ASP:N    | 2.16                     | 0.59              |
| 43:BU:112:ARG:NH2  | 44:BV:46:VAL:HG11  | 2.17                     | 0.59              |
| 47:BY:2:ARG:C      | 47:BY:4:LYS:H      | 2.05                     | 0.59              |
| 47:BY:39:VAL:O     | 47:BY:40:GLU:CG    | 2.48                     | 0.59              |
| 47:BY:7:VAL:CG2    | 47:BY:8:LYS:NZ     | 2.66                     | 0.59              |
| 48:BZ:8:TYR:CE1    | 48:BZ:60:LEU:HD12  | 2.38                     | 0.59              |
| 1:CA:1066:C:H2'    | 1:CA:1067:A:C8     | 2.36                     | 0.59              |
| 1:CA:1318:A:O2'    | 19:CS:37:ARG:HB2   | 2.03                     | 0.59              |
| 1:CA:855:G:O2'     | 1:CA:856:C:H5'     | 2.03                     | 0.59              |
| 2:CB:54:THR:HG23   | 2:CB:199:TYR:HB3   | 1.84                     | 0.59              |
| 4:CD:11:LEU:C      | 4:CD:13:ARG:N      | 2.55                     | 0.59              |
| 7:CG:59:LEU:C      | 7:CG:59:LEU:HD23   | 2.23                     | 0.59              |
| 9:CI:47:LEU:C      | 9:CI:49:PRO:HD2    | 2.21                     | 0.59              |
| 10:CJ:4:ILE:HD12   | 10:CJ:74:ILE:CD1   | 2.33                     | 0.59              |
| 11:CK:103:LEU:HD13 | 11:CK:104:GLN:N    | 2.17                     | 0.59              |
| 17:CQ:16:GLN:O     | 17:CQ:17:LYS:HB2   | 2.01                     | 0.59              |
| 17:CQ:5:VAL:C      | 17:CQ:6:LEU:HD12   | 2.22                     | 0.59              |
| 55:D6:8:LYS:HE3    | 55:D6:8:LYS:O      | 2.03                     | 0.59              |
| 27:DA:1387:C:H2'   | 27:DA:1388:G:H8    | 1.68                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:196:A:H61   | 27:DA:831:G:H21   | 1.51                     | 0.59              |
| 27:DA:2233:U:H2'  | 27:DA:2234:G:H8   | 1.68                     | 0.59              |
| 27:DA:2283:C:C2'  | 27:DA:2284:C:H5'  | 2.32                     | 0.59              |
| 27:DA:2543:G:H2'  | 27:DA:2544:G:H8   | 1.68                     | 0.59              |
| 27:DA:2571:C:H5'' | 27:DA:2572:A:H5'  | 1.84                     | 0.59              |
| 27:DA:2772:C:H2'  | 27:DA:2773:C:H6   | 1.67                     | 0.59              |
| 27:DA:2842:G:C2'  | 27:DA:2843:G:H5'  | 2.32                     | 0.59              |
| 27:DA:479:A:N1    | 27:DA:506:G:N2    | 2.51                     | 0.59              |
| 27:DA:768:G:O2'   | 27:DA:1379:A:N6   | 2.36                     | 0.59              |
| 27:DA:869:G:O2'   | 27:DA:870:A:H5'   | 2.03                     | 0.59              |
| 27:DA:872:A:H61   | 27:DA:905:U:H3    | 1.51                     | 0.59              |
| 31:DE:59:VAL:O    | 31:DE:60:ASN:HB3  | 2.02                     | 0.59              |
| 32:DF:157:VAL:HA  | 32:DF:176:LEU:O   | 2.03                     | 0.59              |
| 35:DI:113:ARG:O   | 35:DI:130:TYR:HD1 | 1.86                     | 0.59              |
| 35:DI:18:VAL:HG12 | 35:DI:18:VAL:O    | 2.01                     | 0.59              |
| 36:DN:21:LYS:HD3  | 36:DN:26:LEU:HD13 | 1.85                     | 0.59              |
| 37:DO:25:LEU:HB2  | 37:DO:38:VAL:O    | 2.03                     | 0.59              |
| 1:AA:288:A:H2'    | 1:AA:289:G:H4'    | 1.84                     | 0.59              |
| 1:AA:313:A:H2'    | 1:AA:314:C:C6     | 2.37                     | 0.59              |
| 1:AA:312:C:H2'    | 1:AA:313:A:H8     | 1.67                     | 0.59              |
| 1:AA:826:C:H2'    | 1:AA:827:U:H6     | 1.67                     | 0.59              |
| 2:AB:63:MET:CB    | 2:AB:225:ALA:HB1  | 2.29                     | 0.59              |
| 3:AC:164:ARG:O    | 3:AC:165:THR:HB   | 2.03                     | 0.59              |
| 5:AE:43:LEU:HD21  | 5:AE:132:ALA:HB1  | 1.83                     | 0.59              |
| 7:AG:11:GLN:HG3   | 7:AG:12:LEU:H     | 1.67                     | 0.59              |
| 2:AB:178:ARG:HH21 | 8:AH:68:ARG:NH2   | 2.01                     | 0.59              |
| 8:AH:74:PRO:HG2   | 8:AH:75:ARG:H     | 1.67                     | 0.59              |
| 9:AI:13:ALA:HB2   | 9:AI:68:GLY:HA3   | 1.84                     | 0.59              |
| 11:AK:84:VAL:C    | 11:AK:85:ARG:HG2  | 2.23                     | 0.59              |
| 11:AK:91:ARG:HD2  | 11:AK:92:GLU:N    | 2.17                     | 0.59              |
| 12:AL:74:LEU:HD21 | 12:AL:104:ALA:HB2 | 1.85                     | 0.59              |
| 12:AL:35:THR:HG21 | 12:AL:62:GLU:OE2  | 2.03                     | 0.59              |
| 14:AN:25:VAL:HB   | 14:AN:38:GLY:O    | 2.03                     | 0.59              |
| 15:AO:17:ARG:NH1  | 15:AO:77:ARG:HH12 | 2.00                     | 0.59              |
| 51:B2:32:LEU:HB2  | 51:B2:53:LEU:HD12 | 1.85                     | 0.59              |
| 27:BA:125:G:N2    | 56:B7:48:LYS:HZ2  | 1.99                     | 0.59              |
| 27:BA:2680:C:H42  | 27:BA:2727:G:H1   | 1.51                     | 0.59              |
| 27:BA:304:G:H2'   | 27:BA:305:U:H6    | 1.65                     | 0.59              |
| 27:BA:542:C:C2'   | 27:BA:543:C:OP1   | 2.51                     | 0.59              |
| 28:BB:105:A:O2'   | 28:BB:106:G:H5'   | 2.02                     | 0.59              |
| 31:BE:35:GLN:HG3  | 31:BE:36:ARG:O    | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BP:149:GLU:HA  | 38:BP:149:GLU:OE2 | 2.03                     | 0.59              |
| 40:BR:21:TYR:HB3  | 40:BR:47:PHE:CD1  | 2.37                     | 0.59              |
| 41:BS:85:VAL:H    | 41:BS:106:ARG:CB  | 2.10                     | 0.59              |
| 44:BV:1:MET:CE    | 44:BV:43:GLU:HG2  | 2.32                     | 0.59              |
| 47:BY:68:HIS:HB2  | 47:BY:71:LYS:HE2  | 1.85                     | 0.59              |
| 48:BZ:18:ARG:HH11 | 48:BZ:81:ARG:NH2  | 2.01                     | 0.59              |
| 1:CA:1498:U:H2'   | 22:CV:5:U:OP1     | 2.03                     | 0.59              |
| 1:CA:908:A:O2'    | 1:CA:909:A:H5'    | 2.02                     | 0.59              |
| 1:CA:971:G:H5''   | 1:CA:972:C:C5'    | 2.31                     | 0.59              |
| 2:CB:130:ARG:HE   | 2:CB:130:ARG:HA   | 1.67                     | 0.59              |
| 25:CY:66:A:H2'    | 25:CY:67:C:C6     | 2.38                     | 0.59              |
| 52:D3:4:LEU:HD23  | 52:D3:57:GLU:O    | 2.03                     | 0.59              |
| 55:D6:15:GLU:CD   | 55:D6:43:CYS:SG   | 2.81                     | 0.59              |
| 27:DA:1203:G:H3'  | 27:DA:1204:A:H5'' | 1.85                     | 0.59              |
| 27:DA:1467:C:H5   | 27:DA:1546:C:H2'  | 1.68                     | 0.59              |
| 27:DA:1668:A:H5'  | 27:DA:1669:A:C5   | 2.37                     | 0.59              |
| 27:DA:1700:A:O2'  | 27:DA:1701:A:O5'  | 2.19                     | 0.59              |
| 27:DA:2172:U:C1'  | 27:DA:2173:A:OP1  | 2.47                     | 0.59              |
| 27:DA:461:C:O2'   | 27:DA:462:C:H5'   | 2.03                     | 0.59              |
| 27:DA:678:C:O2'   | 27:DA:679:C:H5'   | 2.02                     | 0.59              |
| 27:DA:803:U:H6    | 27:DA:803:U:O5'   | 1.84                     | 0.59              |
| 34:DH:156:ALA:C   | 34:DH:158:HIS:H   | 2.05                     | 0.59              |
| 36:DN:87:LEU:O    | 36:DN:87:LEU:HD23 | 2.03                     | 0.59              |
| 37:DO:78:ARG:HH21 | 42:DT:103:ARG:NH2 | 2.00                     | 0.59              |
| 37:DO:86:ILE:N    | 37:DO:86:ILE:HD12 | 2.18                     | 0.59              |
| 32:DF:187:VAL:CB  | 38:DP:7:ARG:HH21  | 2.15                     | 0.59              |
| 38:DP:99:LEU:HG   | 38:DP:102:ARG:NH1 | 2.17                     | 0.59              |
| 39:DQ:55:VAL:CG1  | 39:DQ:56:ARG:H    | 2.13                     | 0.59              |
| 43:DU:21:ALA:O    | 43:DU:24:TYR:CD1  | 2.56                     | 0.59              |
| 43:DU:39:LEU:O    | 43:DU:40:PHE:C    | 2.41                     | 0.59              |
| 27:DA:993:G:OP1   | 43:DU:50:ARG:NH2  | 2.35                     | 0.59              |
| 44:DV:6:LYS:O     | 44:DV:37:VAL:HG21 | 2.02                     | 0.59              |
| 27:DA:2010:G:H5'' | 45:DW:42:ARG:HB2  | 1.83                     | 0.59              |
| 1:AA:434:U:H2'    | 1:AA:435:C:C6     | 2.38                     | 0.59              |
| 1:AA:722:A:O2'    | 1:AA:723:U:H2'    | 2.03                     | 0.59              |
| 1:AA:93:G:N3      | 1:AA:93:G:H2'     | 2.17                     | 0.59              |
| 4:AD:54:TYR:HE1   | 4:AD:209:ARG:HD2  | 1.66                     | 0.59              |
| 1:AA:932:C:C5     | 7:AG:3:ARG:HD3    | 2.37                     | 0.59              |
| 15:AO:54:ARG:NH1  | 15:AO:58:MET:CE   | 2.65                     | 0.59              |
| 24:AX:73:A:H5'    | 24:AX:74:C:OP1    | 2.01                     | 0.59              |
| 49:B0:17:GLN:OE1  | 49:B0:17:GLN:N    | 2.36                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:B3:30:ARG:HD3   | 52:B3:33:GLN:NE2   | 2.18                     | 0.59              |
| 53:B4:48:ILE:HG22  | 53:B4:50:THR:HG23  | 1.83                     | 0.59              |
| 57:B8:32:LEU:HB3   | 57:B8:36:LYS:NZ    | 2.16                     | 0.59              |
| 27:BA:2047:U:O2'   | 27:BA:2048:G:H5''  | 2.03                     | 0.59              |
| 27:BA:2118:U:O2'   | 27:BA:2119:A:C5'   | 2.51                     | 0.59              |
| 27:BA:271(T):C:O2' | 27:BA:271(U):G:H5' | 2.03                     | 0.59              |
| 27:BA:2770:G:H5'   | 27:BA:2771:C:OP2   | 2.03                     | 0.59              |
| 27:BA:519:U:H2'    | 27:BA:520:G:H8     | 1.67                     | 0.59              |
| 27:BA:592:G:N3     | 57:B8:4:MET:HE2    | 2.18                     | 0.59              |
| 27:BA:706:A:C2     | 27:BA:707:G:H1'    | 2.38                     | 0.59              |
| 31:BE:72:VAL:O     | 31:BE:73:GLU:C     | 2.41                     | 0.59              |
| 32:BF:63:LYS:HG2   | 32:BF:65:TRP:O     | 2.03                     | 0.59              |
| 34:BH:43:VAL:HB    | 34:BH:51:ARG:O     | 2.03                     | 0.59              |
| 34:BH:71:LEU:N     | 34:BH:74:ASN:HD22  | 2.01                     | 0.59              |
| 37:BO:35:VAL:HA    | 37:BO:62:VAL:HG12  | 1.84                     | 0.59              |
| 37:BO:16:ALA:CB    | 37:BO:52:VAL:HG11  | 2.31                     | 0.59              |
| 37:BO:7:TYR:CE2    | 37:BO:44:LYS:HG3   | 2.37                     | 0.59              |
| 38:BP:111:ARG:HA   | 38:BP:128:HIS:CD2  | 2.38                     | 0.59              |
| 38:BP:48:PRO:CG    | 38:BP:49:ARG:N     | 2.65                     | 0.59              |
| 40:BR:49:ASP:OD1   | 40:BR:95:THR:HG22  | 2.03                     | 0.59              |
| 46:BX:40:LYS:O     | 46:BX:43:VAL:HB    | 2.03                     | 0.59              |
| 1:CA:1260:C:C6     | 1:CA:1260:C:H3'    | 2.38                     | 0.59              |
| 1:CA:1348:U:OP1    | 9:CI:109:VAL:HA    | 2.02                     | 0.59              |
| 1:CA:1477:C:O2'    | 1:CA:1478:C:H5'    | 2.03                     | 0.59              |
| 1:CA:923:A:OP1     | 5:CE:21:ALA:HB2    | 2.02                     | 0.59              |
| 12:CL:123:LYS:O    | 12:CL:125:ALA:N    | 2.35                     | 0.59              |
| 12:CL:98:VAL:HG12  | 12:CL:101:VAL:HG21 | 1.83                     | 0.59              |
| 1:CA:1060:C:C5'    | 14:CN:45:ARG:HH22  | 2.14                     | 0.59              |
| 27:DA:530:G:N7     | 27:DA:2022:U:H5''  | 2.18                     | 0.59              |
| 27:DA:2494:G:H2'   | 27:DA:2495:G:O5'   | 2.03                     | 0.59              |
| 27:DA:271(H):G:H1  | 27:DA:271(P):C:N4  | 2.00                     | 0.59              |
| 27:DA:675:A:H4'    | 32:DF:67:GLN:OE1   | 2.02                     | 0.59              |
| 27:DA:848:G:O2'    | 27:DA:849:A:H5'    | 2.03                     | 0.59              |
| 27:DA:969:U:H2'    | 27:DA:970:C:C6     | 2.38                     | 0.59              |
| 31:DE:4:ILE:HG12   | 31:DE:28:ALA:CB    | 2.33                     | 0.59              |
| 34:DH:85:LYS:CD    | 34:DH:133:VAL:HB   | 2.32                     | 0.59              |
| 36:DN:118:LYS:C    | 36:DN:120:LEU:H    | 2.05                     | 0.59              |
| 36:DN:42:TRP:HA    | 36:DN:42:TRP:CE3   | 2.37                     | 0.59              |
| 32:DF:187:VAL:HG12 | 38:DP:7:ARG:NH2    | 2.17                     | 0.59              |
| 40:DR:100:LEU:HD21 | 40:DR:113:LEU:HD22 | 1.85                     | 0.59              |
| 40:DR:75:LEU:O     | 40:DR:75:LEU:HD22  | 2.03                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:DS:67:ARG:HG2   | 41:DS:67:ARG:HH11  | 1.68                     | 0.59              |
| 42:DT:104:ASN:O    | 42:DT:105:LEU:HD23 | 2.03                     | 0.59              |
| 42:DT:109:GLU:HG2  | 42:DT:112:ARG:NH1  | 2.17                     | 0.59              |
| 42:DT:83:ILE:CG1   | 42:DT:84:GLN:H     | 2.12                     | 0.59              |
| 27:DA:2018:G:H21   | 43:DU:34:LYS:HZ2   | 1.51                     | 0.59              |
| 1:AA:1363(A):A:H1' | 1:AA:1365:G:N7     | 2.17                     | 0.59              |
| 1:AA:410:G:OP2     | 4:AD:25:ARG:HG3    | 2.03                     | 0.59              |
| 1:AA:655:A:O2'     | 1:AA:656:C:H5'     | 2.03                     | 0.59              |
| 2:AB:140:HIS:HA    | 2:AB:143:GLU:HG3   | 1.84                     | 0.59              |
| 2:AB:115:LEU:HD13  | 2:AB:145:LEU:HB3   | 1.84                     | 0.59              |
| 1:AA:1057:G:H5''   | 3:AC:154:SER:HB2   | 1.85                     | 0.59              |
| 6:AF:86:ARG:O      | 6:AF:87:ARG:HG2    | 2.03                     | 0.59              |
| 9:AI:96:LEU:HD11   | 9:AI:102:LEU:HB2   | 1.84                     | 0.59              |
| 9:AI:7:THR:H       | 9:AI:83:ARG:HD2    | 1.68                     | 0.59              |
| 10:AJ:54:PHE:CD1   | 10:AJ:55:LYS:HE3   | 2.38                     | 0.59              |
| 10:AJ:48:THR:HG23  | 10:AJ:62:HIS:HB3   | 1.84                     | 0.59              |
| 12:AL:114:ARG:HD2  | 12:AL:119:THR:HG21 | 1.84                     | 0.59              |
| 16:AP:26:ARG:NH1   | 16:AP:31:LYS:HB3   | 2.18                     | 0.59              |
| 17:AQ:63:ARG:HG2   | 17:AQ:64:PRO:HD2   | 1.85                     | 0.59              |
| 19:AS:12:ASP:O     | 19:AS:16:LEU:HD13  | 2.03                     | 0.59              |
| 20:AT:26:ASN:ND2   | 20:AT:26:ASN:N     | 2.41                     | 0.59              |
| 25:AY:18:G:H5'     | 25:AY:19:U:C5      | 2.38                     | 0.59              |
| 27:BA:2262:U:OP2   | 49:B0:16:SER:HB2   | 2.03                     | 0.59              |
| 27:BA:1022:G:O2'   | 27:BA:1024:G:N7    | 2.35                     | 0.59              |
| 27:BA:1644:C:O2'   | 27:BA:1645:G:H5'   | 2.02                     | 0.59              |
| 27:BA:1848:A:H2'   | 27:BA:1849:G:C8    | 2.38                     | 0.59              |
| 27:BA:2515:C:O2'   | 27:BA:2516:G:H5'   | 2.03                     | 0.59              |
| 27:BA:2577:A:H5''  | 27:BA:2578:G:H5'   | 1.84                     | 0.59              |
| 27:BA:2626:C:O2'   | 27:BA:2627:G:H5'   | 2.02                     | 0.59              |
| 29:BC:49:ILE:CD1   | 29:BC:49:ILE:H     | 2.13                     | 0.59              |
| 30:BD:131:LEU:N    | 30:BD:131:LEU:HD12 | 2.17                     | 0.59              |
| 31:BE:112:GLY:O    | 31:BE:160:TYR:N    | 2.36                     | 0.59              |
| 31:BE:16:ARG:HG3   | 31:BE:16:ARG:NH1   | 2.18                     | 0.59              |
| 31:BE:56:PRO:HD2   | 31:BE:58:ARG:HG3   | 1.83                     | 0.59              |
| 34:BH:86:GLU:CB    | 34:BH:132:ARG:NH1  | 2.65                     | 0.59              |
| 37:BO:13:ASN:HD21  | 37:BO:96:THR:CA    | 2.16                     | 0.59              |
| 43:BU:92:ARG:CG    | 44:BV:11:GLN:NE2   | 2.65                     | 0.59              |
| 47:BY:67:LEU:HD12  | 47:BY:71:LYS:HE3   | 1.85                     | 0.59              |
| 48:BZ:109:GLY:HA3  | 48:BZ:144:GLU:OE1  | 2.03                     | 0.59              |
| 1:CA:1071:C:H2'    | 1:CA:1072:G:C8     | 2.38                     | 0.59              |
| 1:CA:1441:G:H4'    | 1:CA:1442:G:C8     | 2.38                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:484:G:H4'     | 1:CA:485:G:O5'    | 2.02                     | 0.59              |
| 2:CB:168:THR:HG23  | 2:CB:192:SER:OG   | 2.02                     | 0.59              |
| 3:CC:186:PHE:CZ    | 3:CC:188:LEU:HD22 | 2.38                     | 0.59              |
| 4:CD:61:LYS:NZ     | 4:CD:62:GLN:NE2   | 2.51                     | 0.59              |
| 6:CF:96:PRO:HB3    | 18:CR:30:ASP:CG   | 2.23                     | 0.59              |
| 6:CF:98:LEU:HD12   | 6:CF:98:LEU:N     | 2.16                     | 0.59              |
| 8:CH:89:PRO:HA     | 8:CH:92:ARG:HH11  | 1.67                     | 0.59              |
| 19:CS:52:TYR:HB2   | 19:CS:57:HIS:CE1  | 2.38                     | 0.59              |
| 25:CY:18:G:H22     | 25:CY:55:C:H42    | 1.49                     | 0.59              |
| 25:CY:27:C:H2'     | 25:CY:28:G:H8     | 1.68                     | 0.59              |
| 25:CY:37:U:H2'     | 25:CY:38:U:H5''   | 1.85                     | 0.59              |
| 25:CY:42:G:H2'     | 25:CY:43:C:H5'    | 1.83                     | 0.59              |
| 27:DA:1042:G:H1'   | 27:DA:1114:G:H22  | 1.67                     | 0.59              |
| 27:DA:151:C:O2'    | 27:DA:152:G:H5'   | 2.02                     | 0.59              |
| 27:DA:199:A:N1     | 27:DA:2433:A:H2'  | 2.17                     | 0.59              |
| 27:DA:2533:A:O5'   | 27:DA:2533:A:H8   | 1.86                     | 0.59              |
| 27:DA:2870:C:H2'   | 27:DA:2871:C:C5'  | 2.27                     | 0.59              |
| 27:DA:414:C:O2'    | 27:DA:415:A:H5'   | 2.02                     | 0.59              |
| 27:DA:447:A:N7     | 27:DA:454:A:N6    | 2.50                     | 0.59              |
| 30:DD:223:GLY:O    | 30:DD:225:ALA:N   | 2.36                     | 0.59              |
| 34:DH:150:ALA:C    | 34:DH:152:ARG:H   | 2.06                     | 0.59              |
| 37:DO:65:THR:HA    | 37:DO:82:ASN:HD22 | 1.67                     | 0.59              |
| 27:DA:495:G:H21    | 45:DW:61:ASN:ND2  | 2.01                     | 0.59              |
| 48:DZ:120:HIS:C    | 48:DZ:122:ASP:N   | 2.55                     | 0.59              |
| 1:AA:1022:G:H2'    | 1:AA:1023:G:C8    | 2.38                     | 0.59              |
| 1:AA:1030(D):A:H2' | 1:AA:1031:G:H5'   | 1.85                     | 0.59              |
| 1:AA:113:G:H1'     | 1:AA:354:G:H5'    | 1.84                     | 0.59              |
| 1:AA:38:G:C2       | 1:AA:397:A:C2     | 2.90                     | 0.59              |
| 1:AA:389:A:H2'     | 1:AA:390:C:H5'    | 1.84                     | 0.59              |
| 1:AA:751:U:H4'     | 15:AO:24:SER:CA   | 2.27                     | 0.59              |
| 7:AG:140:ASP:HA    | 7:AG:143:ARG:HH12 | 1.66                     | 0.59              |
| 11:AK:41:THR:HG21  | 11:AK:71:LYS:HB2  | 1.84                     | 0.59              |
| 13:AM:3:ARG:O      | 13:AM:4:ILE:HG13  | 2.03                     | 0.59              |
| 13:AM:65:LYS:HB3   | 13:AM:70:LEU:HB2  | 1.85                     | 0.59              |
| 50:B1:70:VAL:HG12  | 50:B1:71:TYR:N    | 2.18                     | 0.59              |
| 56:B7:8:ASN:HD21   | 56:B7:10:ARG:HB3  | 1.68                     | 0.59              |
| 27:BA:1191:G:OP1   | 38:BP:35:HIS:CE1  | 2.56                     | 0.59              |
| 27:BA:1484:G:H3'   | 27:BA:1485:G:C5'  | 2.27                     | 0.59              |
| 27:BA:1931:U:H2'   | 27:BA:1932:A:C8   | 2.38                     | 0.59              |
| 27:BA:2017:U:O2    | 54:B5:10:LYS:HB2  | 2.02                     | 0.59              |
| 27:BA:2317:C:H2'   | 27:BA:2318:G:C5'  | 2.24                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2327:A:H2'  | 27:BA:2328:A:H8    | 1.60                     | 0.59              |
| 27:BA:553:G:O2'   | 27:BA:554:U:H5'    | 2.03                     | 0.59              |
| 27:BA:88:G:N3     | 27:BA:88:G:H2'     | 2.17                     | 0.59              |
| 30:BD:231:HIS:HD2 | 30:BD:249:PRO:HG3  | 1.67                     | 0.59              |
| 38:BP:16:ARG:HD3  | 38:BP:18:ARG:N     | 2.16                     | 0.59              |
| 38:BP:33:ARG:O    | 38:BP:34:GLY:C     | 2.41                     | 0.59              |
| 41:BS:77:ALA:O    | 41:BS:80:LEU:N     | 2.35                     | 0.59              |
| 43:BU:85:LYS:HD3  | 43:BU:117:GLN:HE22 | 1.67                     | 0.59              |
| 43:BU:35:ALA:O    | 43:BU:39:LEU:HG    | 2.03                     | 0.59              |
| 46:BX:60:ARG:NH1  | 56:B7:47:ARG:NH2   | 2.50                     | 0.59              |
| 1:CA:1002:G:N3    | 1:CA:1002:G:H2'    | 2.18                     | 0.59              |
| 1:CA:1321:C:C5    | 1:CA:1322:C:H2'    | 2.37                     | 0.59              |
| 1:CA:1309:G:O6    | 1:CA:1328:C:N3     | 2.36                     | 0.59              |
| 1:CA:362:G:O5'    | 1:CA:362:G:H8      | 1.85                     | 0.59              |
| 1:CA:874:G:O2'    | 1:CA:875:C:H6      | 1.85                     | 0.59              |
| 3:CC:186:PHE:HD1  | 3:CC:198:VAL:O     | 1.84                     | 0.59              |
| 9:CI:114:TYR:CD2  | 9:CI:114:TYR:N     | 2.65                     | 0.59              |
| 14:CN:3:ARG:O     | 14:CN:7:ILE:HG23   | 2.03                     | 0.59              |
| 14:CN:7:ILE:HG22  | 14:CN:28:GLY:HA3   | 1.83                     | 0.59              |
| 24:CX:12:G:H1'    | 27:DA:1923:U:O2'   | 2.03                     | 0.59              |
| 25:CY:12:C:H2'    | 25:CY:13:A:O4'     | 2.03                     | 0.59              |
| 25:CY:24:C:H2'    | 25:CY:25:A:H8      | 1.68                     | 0.59              |
| 54:D5:56:LYS:HG3  | 54:D5:59:GLU:OE1   | 2.03                     | 0.59              |
| 27:DA:1504:C:H2'  | 27:DA:1505:C:C5'   | 2.28                     | 0.59              |
| 27:DA:249:C:H2'   | 27:DA:249:C:O2     | 2.01                     | 0.59              |
| 27:DA:2551:C:H2'  | 27:DA:2552:U:C6    | 2.38                     | 0.59              |
| 27:DA:2612:C:C4   | 27:DA:2613:U:H5    | 2.20                     | 0.59              |
| 27:DA:262:A:H2'   | 27:DA:263:C:H6     | 1.67                     | 0.59              |
| 27:DA:2697:G:H1   | 27:DA:2710:C:H42   | 1.49                     | 0.59              |
| 27:DA:985:C:O2'   | 27:DA:986:C:H5'    | 2.03                     | 0.59              |
| 29:DC:37:PHE:O    | 29:DC:39:GLU:N     | 2.35                     | 0.59              |
| 30:DD:92:ILE:H    | 30:DD:92:ILE:HD13  | 1.68                     | 0.59              |
| 31:DE:81:ILE:O    | 31:DE:82:ARG:HB2   | 2.03                     | 0.59              |
| 37:DO:35:VAL:HG21 | 37:DO:69:ILE:HD13  | 1.83                     | 0.59              |
| 39:DQ:1:MET:CE    | 39:DQ:44:ALA:HB1   | 2.33                     | 0.59              |
| 40:DR:67:LEU:HD11 | 40:DR:76:VAL:HG21  | 1.84                     | 0.59              |
| 43:DU:55:ARG:CA   | 43:DU:58:ARG:HB2   | 2.20                     | 0.59              |
| 43:DU:89:GLU:HG3  | 44:DV:50:PRO:HG3   | 1.83                     | 0.59              |
| 45:DW:73:ALA:HB3  | 45:DW:106:ILE:HD11 | 1.85                     | 0.59              |
| 45:DW:51:LEU:O    | 45:DW:54:ALA:N     | 2.36                     | 0.59              |
| 46:DX:5:TYR:N     | 46:DX:5:TYR:HD1    | 2.01                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:257:G:H2'     | 1:AA:258:G:H8      | 1.68                     | 0.58              |
| 1:AA:826:C:C2      | 1:AA:827:U:C5      | 2.91                     | 0.58              |
| 1:AA:848:C:H2'     | 1:AA:849:C:H6      | 1.66                     | 0.58              |
| 2:AB:17:PHE:CD1    | 2:AB:44:LEU:HD21   | 2.37                     | 0.58              |
| 2:AB:217:ARG:O     | 2:AB:221:LEU:HD23  | 2.03                     | 0.58              |
| 3:AC:84:ILE:HD13   | 3:AC:88:ARG:NH2    | 2.17                     | 0.58              |
| 7:AG:26:PHE:HB2    | 7:AG:62:PHE:HZ     | 1.67                     | 0.58              |
| 10:AJ:4:ILE:HG12   | 10:AJ:100:THR:HG22 | 1.84                     | 0.58              |
| 11:AK:38:ASN:HD22  | 11:AK:38:ASN:N     | 2.01                     | 0.58              |
| 1:AA:976:G:P       | 14:AN:32:SER:H     | 2.26                     | 0.58              |
| 15:AO:25:THR:HG21  | 15:AO:70:LEU:HB2   | 1.84                     | 0.58              |
| 19:AS:61:TYR:O     | 19:AS:62:ILE:CB    | 2.51                     | 0.58              |
| 21:AU:9:ARG:NH1    | 21:AU:22:ARG:HG3   | 2.18                     | 0.58              |
| 25:AY:51:G:H2'     | 25:AY:52:G:H8      | 1.68                     | 0.58              |
| 54:B5:31:VAL:HB    | 54:B5:32:PRO:HD2   | 1.85                     | 0.58              |
| 27:BA:1479:G:C4    | 27:BA:1480:G:C8    | 2.91                     | 0.58              |
| 27:BA:1811:G:O2'   | 27:BA:1812:A:H5'   | 2.02                     | 0.58              |
| 27:BA:1826:G:H4'   | 30:BD:242:ARG:CZ   | 2.33                     | 0.58              |
| 27:BA:200:U:H5'    | 27:BA:200:U:C6     | 2.30                     | 0.58              |
| 27:BA:2022:U:O2'   | 27:BA:2617:C:H5'   | 2.03                     | 0.58              |
| 27:BA:2778:A:H4'   | 27:BA:2779:U:OP2   | 2.03                     | 0.58              |
| 29:BC:214:VAL:O    | 29:BC:215:THR:C    | 2.40                     | 0.58              |
| 30:BD:75:ILE:O     | 30:BD:118:VAL:HG23 | 2.03                     | 0.58              |
| 31:BE:134:ILE:O    | 31:BE:134:ILE:CG1  | 2.46                     | 0.58              |
| 27:BA:659:C:O2'    | 32:BF:101:LEU:HD12 | 2.03                     | 0.58              |
| 32:BF:112:MET:O    | 32:BF:115:ALA:HB3  | 2.03                     | 0.58              |
| 33:BG:112:PRO:C    | 33:BG:113:ARG:NH1  | 2.50                     | 0.58              |
| 35:BI:101:LEU:HD12 | 35:BI:105:HIS:HB2  | 1.85                     | 0.58              |
| 39:BQ:52:VAL:HA    | 39:BQ:55:VAL:HG13  | 1.84                     | 0.58              |
| 43:BU:20:LEU:HB3   | 43:BU:39:LEU:HD11  | 1.84                     | 0.58              |
| 1:CA:1221:G:H4'    | 19:CS:53:ASN:O     | 2.03                     | 0.58              |
| 1:CA:1302:U:H5     | 13:CM:17:VAL:HG22  | 1.67                     | 0.58              |
| 1:CA:1310:G:H5'    | 13:CM:77:ASN:ND2   | 2.17                     | 0.58              |
| 1:CA:147:G:H1      | 1:CA:175:C:H42     | 1.49                     | 0.58              |
| 1:CA:334:C:O2'     | 1:CA:335:C:H5'     | 2.03                     | 0.58              |
| 1:CA:37:U:H2'      | 1:CA:38:G:H8       | 1.68                     | 0.58              |
| 1:CA:525:C:H5''    | 12:CL:88:LYS:NZ    | 2.18                     | 0.58              |
| 1:CA:793:U:O2      | 1:CA:1516:G:H4'    | 2.03                     | 0.58              |
| 2:CB:144:ARG:HA    | 2:CB:147:LYS:HB3   | 1.83                     | 0.58              |
| 7:CG:109:ASN:HA    | 7:CG:119:ARG:NH1   | 2.18                     | 0.58              |
| 8:CH:20:TYR:HA     | 8:CH:65:TYR:CE2    | 2.37                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:CN:24:CYS:H    | 14:CN:33:VAL:HG11 | 1.68                     | 0.58              |
| 51:D2:21:LEU:HD13 | 51:D2:64:LEU:HA   | 1.85                     | 0.58              |
| 27:DA:1013:C:O2'  | 27:DA:1014:U:H5'  | 2.01                     | 0.58              |
| 27:DA:1050:A:O2'  | 27:DA:1051:G:H8   | 1.85                     | 0.58              |
| 27:DA:1438:U:H5'  | 27:DA:1516:C:O2'  | 2.03                     | 0.58              |
| 27:DA:1484:G:H5'  | 27:DA:1485:G:OP2  | 2.03                     | 0.58              |
| 27:DA:1810:A:H2'  | 27:DA:1811:G:O4'  | 2.03                     | 0.58              |
| 27:DA:2015:A:C2   | 54:D5:6:VAL:HG22  | 2.37                     | 0.58              |
| 27:DA:2092:U:C4   | 27:DA:2226:C:OP2  | 2.56                     | 0.58              |
| 27:DA:2141:G:O2'  | 27:DA:2142:C:H5'  | 2.03                     | 0.58              |
| 27:DA:42:G:H1     | 27:DA:436:C:N4    | 2.01                     | 0.58              |
| 27:DA:863:A:H2'   | 27:DA:864:G:H8    | 1.64                     | 0.58              |
| 27:DA:902:C:H2'   | 27:DA:903:C:H6    | 1.68                     | 0.58              |
| 33:DG:76:SER:CB   | 33:DG:83:ARG:HB2  | 2.33                     | 0.58              |
| 27:DA:2667:C:H1'  | 34:DH:109:PHE:HD2 | 1.68                     | 0.58              |
| 38:DP:87:ASP:C    | 38:DP:89:ALA:H    | 2.07                     | 0.58              |
| 40:DR:77:ARG:C    | 40:DR:79:LEU:N    | 2.57                     | 0.58              |
| 42:DT:30:VAL:HG21 | 42:DT:83:ILE:HG13 | 1.84                     | 0.58              |
| 45:DW:23:LEU:HD21 | 45:DW:39:THR:HG21 | 1.84                     | 0.58              |
| 48:DZ:75:LEU:HD13 | 48:DZ:82:PRO:HA   | 1.85                     | 0.58              |
| 1:AA:1028:C:H42   | 1:AA:1034:G:H21   | 1.50                     | 0.58              |
| 1:AA:1255:G:O3'   | 1:AA:1258:G:H1'   | 2.03                     | 0.58              |
| 1:AA:1426:C:H2'   | 1:AA:1427:U:C6    | 2.37                     | 0.58              |
| 1:AA:563:A:H2'    | 1:AA:563:A:N3     | 2.19                     | 0.58              |
| 1:AA:851:G:H2'    | 1:AA:852:G:H8     | 1.68                     | 0.58              |
| 1:AA:574:A:N3     | 1:AA:883:C:H1'    | 2.18                     | 0.58              |
| 9:AI:96:LEU:CD1   | 9:AI:102:LEU:HB2  | 2.33                     | 0.58              |
| 12:AL:119:THR:CG2 | 12:AL:120:LYS:N   | 2.65                     | 0.58              |
| 12:AL:68:PRO:HG3  | 12:AL:96:HIS:CD2  | 2.38                     | 0.58              |
| 1:AA:1060:C:H5'   | 14:AN:45:ARG:NH2  | 2.18                     | 0.58              |
| 16:AP:20:VAL:HG22 | 16:AP:21:VAL:N    | 2.17                     | 0.58              |
| 19:AS:32:LYS:HB3  | 19:AS:57:HIS:CE1  | 2.38                     | 0.58              |
| 24:AX:58:A:H4'    | 24:AX:59:A:OP1    | 2.03                     | 0.58              |
| 50:B1:64:ALA:HA   | 50:B1:67:ILE:CD1  | 2.33                     | 0.58              |
| 27:BA:2377:A:H4'  | 41:BS:107:GLU:HB3 | 1.84                     | 0.58              |
| 27:BA:246:C:N4    | 57:B8:8:LYS:HG2   | 2.17                     | 0.58              |
| 27:BA:406:G:H1    | 27:BA:421:U:H3    | 1.51                     | 0.58              |
| 27:BA:519:U:H2'   | 27:BA:520:G:C8    | 2.38                     | 0.58              |
| 27:BA:673:C:C6    | 27:BA:673:C:H5''  | 2.37                     | 0.58              |
| 32:BF:46:ARG:HB3  | 32:BF:48:THR:CG2  | 2.34                     | 0.58              |
| 36:BN:62:VAL:HG11 | 36:BN:67:LEU:CG   | 2.33                     | 0.58              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 42:BT:79:HIS:O      | 42:BT:81:PRO:CD   | 2.40                     | 0.58              |
| 44:BV:2:PHE:O       | 44:BV:14:VAL:O    | 2.22                     | 0.58              |
| 45:BW:68:ARG:HH12   | 45:BW:111:HIS:CD2 | 2.21                     | 0.58              |
| 45:BW:13:SER:O      | 45:BW:16:LYS:HB2  | 2.02                     | 0.58              |
| 47:BY:88:LYS:O      | 47:BY:90:LEU:HG   | 2.03                     | 0.58              |
| 1:CA:1469:G:H2'     | 1:CA:1470:G:C8    | 2.38                     | 0.58              |
| 1:CA:353:A:H5'      | 1:CA:353:A:H8     | 1.68                     | 0.58              |
| 3:CC:34:LEU:HD23    | 3:CC:35:GLU:N     | 2.18                     | 0.58              |
| 11:CK:125:PHE:H     | 11:CK:125:PHE:HD1 | 1.51                     | 0.58              |
| 13:CM:88:ARG:HA     | 13:CM:98:VAL:HG12 | 1.84                     | 0.58              |
| 15:CO:82:ILE:O      | 15:CO:82:ILE:HD13 | 2.03                     | 0.58              |
| 53:D4:44:CYS:SG     | 53:D4:44:CYS:O    | 2.61                     | 0.58              |
| 54:D5:45:VAL:O      | 54:D5:46:CYS:C    | 2.41                     | 0.58              |
| 27:DA:1472:A:H2'    | 27:DA:1473:G:O4'  | 2.03                     | 0.58              |
| 27:DA:1631(A):A:O2' | 27:DA:1632:A:H5'  | 2.03                     | 0.58              |
| 27:DA:1655:A:H3'    | 27:DA:1656:C:H6   | 1.68                     | 0.58              |
| 27:DA:2403:C:N3     | 27:DA:2415:G:C2   | 2.71                     | 0.58              |
| 27:DA:2830:G:O2'    | 27:DA:2831:G:H5'  | 2.03                     | 0.58              |
| 27:DA:918:A:C2      | 27:DA:919:G:H1'   | 2.38                     | 0.58              |
| 31:DE:55:ASN:O      | 31:DE:57:LYS:N    | 2.35                     | 0.58              |
| 32:DF:167:ALA:HB1   | 32:DF:173:VAL:CG1 | 2.33                     | 0.58              |
| 34:DH:157:TYR:O     | 34:DH:158:HIS:HB2 | 2.03                     | 0.58              |
| 36:DN:30:ILE:HG23   | 36:DN:52:VAL:HG11 | 1.85                     | 0.58              |
| 41:DS:17:ARG:HA     | 41:DS:20:ARG:CZ   | 2.33                     | 0.58              |
| 42:DT:60:THR:O      | 42:DT:61:PHE:HB3  | 2.01                     | 0.58              |
| 1:AA:1168:A:H2'     | 1:AA:1169:A:C8    | 2.38                     | 0.58              |
| 1:AA:1325:C:H4'     | 21:AU:17:THR:HG21 | 1.86                     | 0.58              |
| 1:AA:1424:C:N4      | 1:AA:1476:G:H1    | 1.98                     | 0.58              |
| 1:AA:460:G:O6       | 1:AA:470:C:H5''   | 2.02                     | 0.58              |
| 1:AA:489:C:H2'      | 1:AA:490:G:H8     | 1.68                     | 0.58              |
| 1:AA:530:G:O2'      | 1:AA:531:U:OP2    | 2.19                     | 0.58              |
| 3:AC:84:ILE:HA      | 3:AC:87:LEU:HD12  | 1.84                     | 0.58              |
| 4:AD:98:GLU:C       | 4:AD:100:ARG:H    | 2.05                     | 0.58              |
| 12:AL:3:THR:N       | 12:AL:6:GLN:HE21  | 2.00                     | 0.58              |
| 12:AL:3:THR:HG23    | 12:AL:6:GLN:NE2   | 2.18                     | 0.58              |
| 1:AA:1330:U:OP1     | 13:AM:22:ILE:O    | 2.21                     | 0.58              |
| 17:AQ:69:LYS:C      | 17:AQ:70:ARG:HD2  | 2.24                     | 0.58              |
| 23:AW:18:G:H1'      | 23:AW:19:U:O2     | 2.03                     | 0.58              |
| 53:B4:40:ILE:HG23   | 53:B4:59:VAL:HG21 | 1.85                     | 0.58              |
| 57:B8:37:SER:OG     | 57:B8:39:LYS:HB3  | 2.04                     | 0.58              |
| 27:BA:1315:C:C2'    | 27:BA:1316:U:H5'  | 2.33                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1698:A:O4'   | 27:BA:1700:A:H4'   | 2.03                     | 0.58              |
| 27:BA:2171:A:O2'   | 27:BA:2172:U:O5'   | 2.19                     | 0.58              |
| 27:BA:2756:U:H5''  | 58:B9:19:ARG:HB3   | 1.86                     | 0.58              |
| 27:BA:709:U:N3     | 27:BA:710:G:N7     | 2.50                     | 0.58              |
| 27:BA:786:C:C4     | 27:BA:787:U:C5     | 2.90                     | 0.58              |
| 28:BB:91:C:C2'     | 28:BB:92:C:O5'     | 2.50                     | 0.58              |
| 27:BA:607:U:P      | 32:BF:103:LYS:HG3  | 2.42                     | 0.58              |
| 32:BF:154:VAL:HG22 | 32:BF:191:ARG:HB2  | 1.85                     | 0.58              |
| 32:BF:20:LEU:HD13  | 32:BF:203:GLN:NE2  | 2.16                     | 0.58              |
| 38:BP:59:LEU:CA    | 38:BP:61:ARG:CZ    | 2.55                     | 0.58              |
| 39:BQ:19:GLY:O     | 39:BQ:20:ALA:HB3   | 2.04                     | 0.58              |
| 42:BT:65:LYS:HG3   | 42:BT:66:VAL:N     | 2.19                     | 0.58              |
| 47:BY:46:LYS:HE2   | 47:BY:47:LYS:HE3   | 1.84                     | 0.58              |
| 47:BY:77:PRO:O     | 47:BY:78:ALA:HB2   | 2.02                     | 0.58              |
| 1:CA:1256:A:N6     | 1:CA:1278:U:O2     | 2.35                     | 0.58              |
| 1:CA:189(D):C:H2'  | 1:CA:189(E):U:O4'  | 2.02                     | 0.58              |
| 1:CA:232:G:H2'     | 1:CA:233:C:C6      | 2.39                     | 0.58              |
| 1:CA:59:A:H4'      | 1:CA:388:G:OP1     | 2.04                     | 0.58              |
| 1:CA:60:A:H5''     | 1:CA:331:G:N2      | 2.18                     | 0.58              |
| 2:CB:67:THR:O      | 2:CB:68:ILE:HD13   | 2.03                     | 0.58              |
| 13:CM:58:GLU:O     | 13:CM:62:ASN:OD1   | 2.22                     | 0.58              |
| 16:CP:58:TYR:O     | 16:CP:60:LEU:N     | 2.37                     | 0.58              |
| 17:CQ:62:SER:HB2   | 17:CQ:72:ARG:HG3   | 1.85                     | 0.58              |
| 20:CT:79:ARG:O     | 20:CT:80:ARG:C     | 2.42                     | 0.58              |
| 50:D1:24:ALA:HB3   | 50:D1:27:GLU:OE2   | 2.03                     | 0.58              |
| 51:D2:49:LYS:O     | 51:D2:52:ASP:HB2   | 2.03                     | 0.58              |
| 56:D7:12:ARG:HD3   | 56:D7:46:VAL:HG21  | 1.84                     | 0.58              |
| 27:DA:1336:A:H2'   | 27:DA:1337:G:H8    | 1.68                     | 0.58              |
| 27:DA:1515:G:H2'   | 27:DA:1516:C:H5'   | 1.86                     | 0.58              |
| 27:DA:1947:C:N4    | 27:DA:1959:G:H1    | 1.99                     | 0.58              |
| 27:DA:220:G:H22    | 27:DA:427:U:H2'    | 1.68                     | 0.58              |
| 27:DA:399:G:O2'    | 27:DA:400:G:H5'    | 2.04                     | 0.58              |
| 27:DA:531:C:C5     | 27:DA:2035:G:C2    | 2.92                     | 0.58              |
| 27:DA:862:G:H21    | 28:DB:101:G:H1'    | 1.67                     | 0.58              |
| 30:DD:228:PRO:HD3  | 30:DD:235:GLY:N    | 2.19                     | 0.58              |
| 30:DD:241:PRO:O    | 30:DD:242:ARG:C    | 2.40                     | 0.58              |
| 30:DD:261:LYS:HZ1  | 30:DD:263:ARG:HH12 | 1.50                     | 0.58              |
| 33:DG:126:ASP:C    | 33:DG:128:ARG:H    | 2.06                     | 0.58              |
| 36:DN:16:ILE:HG23  | 36:DN:54:VAL:HG23  | 1.86                     | 0.58              |
| 27:DA:627:A:N6     | 38:DP:84:ASN:HD21  | 2.00                     | 0.58              |
| 27:DA:2334:G:O2'   | 41:DS:18:ILE:HG21  | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:DU:76:TYR:C    | 43:DU:78:THR:H    | 2.07                     | 0.58              |
| 43:DU:95:LEU:HD13 | 44:DV:4:ILE:HG23  | 1.86                     | 0.58              |
| 45:DW:43:GLY:O    | 45:DW:47:VAL:HG23 | 2.03                     | 0.58              |
| 46:DX:12:VAL:CG2  | 46:DX:13:LEU:H    | 1.89                     | 0.58              |
| 48:DZ:117:GLN:HG2 | 48:DZ:118:GLU:H   | 1.68                     | 0.58              |
| 48:DZ:6:ALA:CB    | 48:DZ:58:LEU:HB3  | 2.32                     | 0.58              |
| 1:AA:144:G:H2'    | 1:AA:145:G:H8     | 1.69                     | 0.58              |
| 1:AA:312:C:H2'    | 1:AA:313:A:C8     | 2.39                     | 0.58              |
| 1:AA:806:C:H2'    | 1:AA:807:A:H8     | 1.67                     | 0.58              |
| 6:AF:62:TRP:HH2   | 6:AF:64:GLN:HB2   | 1.60                     | 0.58              |
| 13:AM:91:ARG:HH22 | 13:AM:103:THR:CG2 | 2.16                     | 0.58              |
| 18:AR:53:ARG:NH1  | 18:AR:53:ARG:HG2  | 2.17                     | 0.58              |
| 53:B4:42:CYS:SG   | 53:B4:62:CYS:HB3  | 2.43                     | 0.58              |
| 53:B4:62:CYS:SG   | 53:B4:64:LYS:HB2  | 2.43                     | 0.58              |
| 54:B5:50:GLY:HA3  | 54:B5:56:LYS:HB3  | 1.85                     | 0.58              |
| 27:BA:1907:G:O2'  | 27:BA:1908:C:H5'  | 2.03                     | 0.58              |
| 27:BA:812:C:OP1   | 27:BA:1251:C:H5'  | 2.03                     | 0.58              |
| 35:BI:113:ARG:O   | 35:BI:130:TYR:HA  | 2.04                     | 0.58              |
| 39:BQ:135:ASP:C   | 39:BQ:137:TYR:N   | 2.54                     | 0.58              |
| 42:BT:23:ARG:HA   | 42:BT:52:ILE:CD1  | 2.33                     | 0.58              |
| 47:BY:2:ARG:CD    | 47:BY:3:VAL:HG23  | 2.32                     | 0.58              |
| 47:BY:6:HIS:ND1   | 47:BY:6:HIS:N     | 2.51                     | 0.58              |
| 1:CA:735:C:H2'    | 1:CA:736:C:C6     | 2.30                     | 0.58              |
| 1:CA:979:C:C5     | 1:CA:980:C:H6     | 2.20                     | 0.58              |
| 4:CD:68:TYR:O     | 4:CD:70:ILE:N     | 2.37                     | 0.58              |
| 5:CE:148:VAL:HG12 | 5:CE:152:ARG:HE   | 1.67                     | 0.58              |
| 8:CH:37:ARG:O     | 8:CH:40:ALA:HB3   | 2.04                     | 0.58              |
| 9:CI:79:LEU:CD2   | 9:CI:102:LEU:HA   | 2.33                     | 0.58              |
| 11:CK:69:ALA:HB1  | 11:CK:73:MET:HE2  | 1.85                     | 0.58              |
| 24:CX:56:C:H2'    | 24:CX:57:A:C8     | 2.38                     | 0.58              |
| 50:D1:7:ILE:HB    | 50:D1:62:VAL:CG2  | 2.34                     | 0.58              |
| 51:D2:16:LEU:H    | 51:D2:67:LYS:HZ1  | 1.51                     | 0.58              |
| 52:D3:7:LYS:CG    | 52:D3:8:LEU:H     | 2.13                     | 0.58              |
| 27:DA:1614:A:H2'  | 27:DA:1615:C:H5'  | 1.85                     | 0.58              |
| 27:DA:1934:C:H2'  | 27:DA:1935:G:H8   | 1.67                     | 0.58              |
| 27:DA:2114:A:H2   | 27:DA:2168:G:O4'  | 1.86                     | 0.58              |
| 27:DA:2111:C:H42  | 27:DA:2147:G:N2   | 2.00                     | 0.58              |
| 27:DA:1805:U:H5'' | 30:DD:250:TRP:CD2 | 2.37                     | 0.58              |
| 30:DD:89:SER:HB2  | 30:DD:159:ALA:HB2 | 1.85                     | 0.58              |
| 31:DE:37:ARG:HB2  | 31:DE:46:ALA:N    | 2.18                     | 0.58              |
| 32:DF:36:VAL:O    | 32:DF:39:TRP:HB3  | 2.04                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DI:107:VAL:CG1  | 35:DI:108:THR:H    | 2.12                     | 0.58              |
| 38:DP:39:LYS:CA    | 38:DP:39:LYS:HE2   | 2.29                     | 0.58              |
| 32:DF:187:VAL:HB   | 38:DP:7:ARG:HH21   | 1.68                     | 0.58              |
| 41:DS:97:ARG:NH2   | 41:DS:99:LYS:H     | 2.00                     | 0.58              |
| 42:DT:88:ILE:CG2   | 42:DT:89:VAL:H     | 1.98                     | 0.58              |
| 46:DX:25:LYS:HZ1   | 46:DX:80:ILE:HD11  | 1.66                     | 0.58              |
| 46:DX:10:ALA:O     | 46:DX:28:PHE:HB3   | 2.02                     | 0.58              |
| 1:AA:501:C:O2'     | 1:AA:502:G:H5'     | 2.03                     | 0.58              |
| 1:AA:723:U:O2'     | 1:AA:724:G:C5'     | 2.51                     | 0.58              |
| 1:AA:909:A:H2'     | 1:AA:910:C:H5'     | 1.84                     | 0.58              |
| 3:AC:140:ARG:HH11  | 3:AC:140:ARG:HG3   | 1.69                     | 0.58              |
| 3:AC:7:PRO:O       | 3:AC:11:ARG:CG     | 2.51                     | 0.58              |
| 5:AE:72:GLN:NE2    | 5:AE:144:THR:HG22  | 2.19                     | 0.58              |
| 6:AF:53:ALA:HB3    | 6:AF:86:ARG:CZ     | 2.33                     | 0.58              |
| 1:AA:963:G:H21     | 10:AJ:55:LYS:NZ    | 2.01                     | 0.58              |
| 51:B2:7:ARG:O      | 51:B2:11:GLU:HG3   | 2.04                     | 0.58              |
| 52:B3:30:ARG:HD3   | 52:B3:30:ARG:H     | 1.68                     | 0.58              |
| 27:BA:1179:C:H2'   | 27:BA:1180:C:H6    | 1.69                     | 0.58              |
| 27:BA:146:G:C2'    | 27:BA:147:U:H5'    | 2.33                     | 0.58              |
| 27:BA:1678:G:N2    | 27:BA:1989:G:H22   | 2.02                     | 0.58              |
| 27:BA:2012:G:O3'   | 45:BW:96:ILE:CD1   | 2.48                     | 0.58              |
| 27:BA:2431:U:O2    | 27:BA:2433:A:C8    | 2.56                     | 0.58              |
| 27:BA:608:A:P      | 32:BF:100:THR:HG21 | 2.43                     | 0.58              |
| 27:BA:848:G:H5'    | 27:BA:848:G:H8     | 1.69                     | 0.58              |
| 31:BE:101:ARG:NH2  | 31:BE:171:GLU:HB2  | 2.17                     | 0.58              |
| 32:BF:123:LEU:HD13 | 32:BF:192:LEU:HD22 | 1.84                     | 0.58              |
| 41:BS:106:ARG:CZ   | 41:BS:107:GLU:O    | 2.52                     | 0.58              |
| 43:BU:101:ARG:C    | 43:BU:102:GLU:HG2  | 2.23                     | 0.58              |
| 48:BZ:107:PRO:HG3  | 48:BZ:116:LEU:HB2  | 1.86                     | 0.58              |
| 1:CA:1116:C:C2'    | 1:CA:1117:G:H5''   | 2.33                     | 0.58              |
| 1:CA:1198:G:H2'    | 1:CA:1199:U:C6     | 2.38                     | 0.58              |
| 1:CA:1246:C:O2'    | 1:CA:1247:U:H5'    | 2.03                     | 0.58              |
| 1:CA:219:C:H2'     | 1:CA:220:G:O4'     | 2.04                     | 0.58              |
| 1:CA:686:U:H3      | 1:CA:703:G:N2      | 2.00                     | 0.58              |
| 1:CA:722:A:N3      | 1:CA:722:A:H2'     | 2.17                     | 0.58              |
| 2:CB:215:LEU:O     | 2:CB:219:VAL:HG23  | 2.03                     | 0.58              |
| 5:CE:102:ALA:HB1   | 5:CE:106:PRO:HG2   | 1.85                     | 0.58              |
| 8:CH:7:ALA:HB2     | 8:CH:85:ARG:HG3    | 1.86                     | 0.58              |
| 17:CQ:94:ASN:O     | 17:CQ:98:LEU:HD12  | 2.03                     | 0.58              |
| 50:D1:6:GLU:O      | 50:D1:7:ILE:HD12   | 2.04                     | 0.58              |
| 27:DA:1252:G:H8    | 27:DA:1252:G:OP1   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2126:A:H5''  | 29:DC:36:LYS:CE    | 2.30                     | 0.58              |
| 27:DA:2262:U:H2'   | 27:DA:2263:C:C6    | 2.38                     | 0.58              |
| 27:DA:635:C:H2'    | 27:DA:636:G:C8     | 2.38                     | 0.58              |
| 27:DA:704:G:H1'    | 27:DA:727:A:H62    | 1.68                     | 0.58              |
| 27:DA:850:C:H2'    | 27:DA:851:U:C6     | 2.38                     | 0.58              |
| 31:DE:110:GLY:O    | 40:DR:2:ARG:CZ     | 2.51                     | 0.58              |
| 31:DE:116:VAL:HG21 | 31:DE:122:PHE:CD2  | 2.38                     | 0.58              |
| 33:DG:57:ALA:HB2   | 33:DG:90:LEU:HD11  | 1.84                     | 0.58              |
| 34:DH:54:ARG:O     | 34:DH:54:ARG:HG3   | 2.03                     | 0.58              |
| 36:DN:22:THR:HA    | 36:DN:60:ILE:CG2   | 2.33                     | 0.58              |
| 37:DO:53:LYS:O     | 37:DO:55:GLY:N     | 2.36                     | 0.58              |
| 27:DA:1244:G:H4'   | 38:DP:11:GLY:CA    | 2.30                     | 0.58              |
| 38:DP:83:VAL:HG23  | 38:DP:87:ASP:OD2   | 2.02                     | 0.58              |
| 42:DT:16:ARG:O     | 42:DT:17:THR:CB    | 2.50                     | 0.58              |
| 1:AA:203:U:H6      | 1:AA:203:U:OP2     | 1.87                     | 0.58              |
| 1:AA:642:A:H2'     | 1:AA:643:C:C6      | 2.38                     | 0.58              |
| 1:AA:711:G:H2'     | 1:AA:712:A:H8      | 1.69                     | 0.58              |
| 3:AC:38:ARG:HD3    | 3:AC:94:LEU:HD22   | 1.85                     | 0.58              |
| 3:AC:47:LEU:O      | 3:AC:47:LEU:HD12   | 2.02                     | 0.58              |
| 1:AA:875:C:O2      | 8:AH:15:ASN:ND2    | 2.32                     | 0.58              |
| 10:AJ:3:LYS:O      | 10:AJ:100:THR:HG22 | 2.03                     | 0.58              |
| 13:AM:100:GLY:C    | 13:AM:101:GLN:HG3  | 2.24                     | 0.58              |
| 49:B0:31:VAL:HB    | 49:B0:35:ASN:ND2   | 2.18                     | 0.58              |
| 50:B1:19:GLN:NE2   | 50:B1:19:GLN:CA    | 2.65                     | 0.58              |
| 27:BA:1021:A:C8    | 27:BA:1021:A:C3'   | 2.80                     | 0.58              |
| 27:BA:1114:G:C2'   | 27:BA:1115:G:H5''  | 2.34                     | 0.58              |
| 27:BA:1607:C:C4'   | 27:BA:1608:A:O5'   | 2.51                     | 0.58              |
| 27:BA:518:G:H2'    | 27:BA:519:U:C5     | 2.38                     | 0.58              |
| 34:BH:121:ILE:HD12 | 34:BH:144:VAL:HG21 | 1.86                     | 0.58              |
| 36:BN:125:GLY:HA3  | 36:BN:126:PRO:O    | 2.04                     | 0.58              |
| 28:BB:7:G:N2       | 41:BS:38:GLN:HE22  | 2.01                     | 0.58              |
| 43:BU:13:LYS:O     | 43:BU:16:LYS:HB3   | 2.04                     | 0.58              |
| 46:BX:63:LYS:HE3   | 46:BX:72:LYS:CE    | 2.24                     | 0.58              |
| 1:CA:1071:C:H2'    | 1:CA:1072:G:H8     | 1.68                     | 0.58              |
| 1:CA:1119:C:O5'    | 1:CA:1119:C:H6     | 1.87                     | 0.58              |
| 1:CA:31:G:H22      | 1:CA:47:C:H4'      | 1.68                     | 0.58              |
| 1:CA:739:C:O2      | 15:CO:42:HIS:HE1   | 1.87                     | 0.58              |
| 1:CA:771:G:O2'     | 1:CA:772:U:H5'     | 2.03                     | 0.58              |
| 4:CD:150:GLU:O     | 4:CD:153:ARG:HG3   | 2.04                     | 0.58              |
| 4:CD:203:VAL:O     | 4:CD:206:PHE:HB3   | 2.04                     | 0.58              |
| 6:CF:72:VAL:HG22   | 6:CF:72:VAL:O      | 2.02                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:CS:32:LYS:CE   | 19:CS:32:LYS:N     | 2.65                     | 0.58              |
| 20:CT:54:LYS:HA   | 20:CT:57:ARG:HH22  | 1.69                     | 0.58              |
| 27:DA:1037:G:H1   | 27:DA:1118:C:H42   | 1.51                     | 0.58              |
| 27:DA:1164:G:H2'  | 27:DA:1165:U:H6    | 1.67                     | 0.58              |
| 27:DA:1317:A:H2'  | 27:DA:1318:C:C6    | 2.39                     | 0.58              |
| 27:DA:1602:U:H3'  | 27:DA:1603:A:H5''  | 1.83                     | 0.58              |
| 27:DA:1655:A:H2'  | 27:DA:1656:C:O4'   | 2.04                     | 0.58              |
| 27:DA:1790:C:H5'' | 27:DA:1791:A:OP1   | 2.03                     | 0.58              |
| 27:DA:2125:G:N2   | 27:DA:2174:C:N4    | 2.52                     | 0.58              |
| 27:DA:2311:A:H5'' | 27:DA:2312:U:OP2   | 2.03                     | 0.58              |
| 27:DA:2371:G:H4'  | 55:D6:45:LYS:CB    | 2.34                     | 0.58              |
| 27:DA:275:G:O3'   | 27:DA:279:C:P      | 2.61                     | 0.58              |
| 27:DA:350:U:H2'   | 27:DA:351:G:O4'    | 2.03                     | 0.58              |
| 27:DA:389:G:H8    | 27:DA:389:G:O5'    | 1.87                     | 0.58              |
| 27:DA:750:A:H2'   | 27:DA:750:A:N3     | 2.18                     | 0.58              |
| 27:DA:817:C:H2'   | 27:DA:818:G:O4'    | 2.03                     | 0.58              |
| 28:DB:103:G:O2'   | 28:DB:104:U:H5'    | 2.03                     | 0.58              |
| 34:DH:27:LYS:HG2  | 34:DH:32:GLU:HB2   | 1.84                     | 0.58              |
| 35:DI:129:THR:O   | 35:DI:130:TYR:CB   | 2.52                     | 0.58              |
| 35:DI:77:LEU:O    | 35:DI:140:LEU:HD12 | 2.02                     | 0.58              |
| 36:DN:35:ARG:O    | 36:DN:49:GLY:HA2   | 2.03                     | 0.58              |
| 42:DT:31:SER:HB2  | 42:DT:32:TYR:CD2   | 2.38                     | 0.58              |
| 44:DV:95:LEU:HD22 | 44:DV:97:LYS:HZ3   | 1.66                     | 0.58              |
| 1:AA:954:G:H21    | 1:AA:1227:A:N6     | 2.00                     | 0.58              |
| 1:AA:198:G:H2'    | 1:AA:199:G:C8      | 2.39                     | 0.58              |
| 1:AA:300:A:H2'    | 1:AA:301:G:O4'     | 2.01                     | 0.58              |
| 1:AA:321:A:C2     | 1:AA:333:G:C2      | 2.92                     | 0.58              |
| 1:AA:37:U:H3      | 1:AA:397:A:H61     | 1.52                     | 0.58              |
| 1:AA:663:A:O2'    | 1:AA:664:G:H5'     | 2.03                     | 0.58              |
| 1:AA:921:U:O2     | 5:AE:19:MET:HB2    | 2.04                     | 0.58              |
| 1:AA:971:G:N2     | 1:AA:1363(A):A:OP2 | 2.34                     | 0.58              |
| 5:AE:11:ILE:HG21  | 5:AE:105:VAL:CG2   | 2.33                     | 0.58              |
| 11:AK:42:TRP:O    | 11:AK:43:SER:HB2   | 2.02                     | 0.58              |
| 12:AL:40:VAL:HG23 | 12:AL:41:THR:N     | 2.17                     | 0.58              |
| 13:AM:27:LYS:HE3  | 13:AM:31:LYS:HE3   | 1.84                     | 0.58              |
| 17:AQ:27:PHE:CD1  | 17:AQ:28:PRO:O     | 2.56                     | 0.58              |
| 6:AF:50:TYR:OH    | 18:AR:74:ARG:O     | 2.14                     | 0.58              |
| 25:AY:51:G:H2'    | 25:AY:52:G:C8      | 2.38                     | 0.58              |
| 27:BA:1293:C:H2'  | 27:BA:1294:U:H6    | 1.68                     | 0.58              |
| 27:BA:154(A):C:N4 | 27:BA:172:C:H42    | 1.96                     | 0.58              |
| 27:BA:2048:G:H2'  | 27:BA:2049:G:O4'   | 2.04                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2088:G:C6   | 27:BA:2089:U:C4    | 2.92                     | 0.58              |
| 27:BA:2690:C:N4   | 27:BA:2713:A:O2'   | 2.36                     | 0.58              |
| 27:BA:2809:A:C2   | 27:BA:2892:A:N3    | 2.72                     | 0.58              |
| 30:BD:209:ALA:O   | 30:BD:213:ARG:HG2  | 2.03                     | 0.58              |
| 31:BE:71:GLY:O    | 31:BE:72:VAL:C     | 2.41                     | 0.58              |
| 36:BN:93:THR:O    | 36:BN:94:HIS:HB2   | 2.04                     | 0.58              |
| 31:BE:52:LEU:HG   | 42:BT:1:MET:HE1    | 1.84                     | 0.58              |
| 47:BY:95:LYS:HG2  | 47:BY:100:ALA:HA   | 1.85                     | 0.58              |
| 1:CA:475:G:H2'    | 1:CA:476:G:C8      | 2.35                     | 0.58              |
| 1:CA:904:C:H2'    | 1:CA:905:U:C6      | 2.38                     | 0.58              |
| 2:CB:97:TRP:HH2   | 2:CB:176:GLU:CD    | 2.06                     | 0.58              |
| 4:CD:61:LYS:HZ3   | 4:CD:62:GLN:NE2    | 2.02                     | 0.58              |
| 4:CD:15:GLU:OE2   | 4:CD:66:ARG:NH1    | 2.37                     | 0.58              |
| 5:CE:20:GLN:O     | 5:CE:21:ALA:O      | 2.21                     | 0.58              |
| 8:CH:10:LEU:HD23  | 8:CH:83:ILE:CG1    | 2.31                     | 0.58              |
| 10:CJ:5:ARG:HD2   | 10:CJ:7:LYS:HE2    | 1.84                     | 0.58              |
| 13:CM:66:LEU:HA   | 13:CM:70:LEU:HB2   | 1.85                     | 0.58              |
| 13:CM:96:LEU:C    | 13:CM:110:ARG:HD3  | 2.23                     | 0.58              |
| 14:CN:21:TYR:HD2  | 14:CN:22:THR:O     | 1.87                     | 0.58              |
| 14:CN:47:LEU:HB2  | 14:CN:53:LEU:HD11  | 1.86                     | 0.58              |
| 15:CO:12:ILE:C    | 15:CO:14:GLU:H     | 2.05                     | 0.58              |
| 16:CP:52:ASP:OD1  | 16:CP:55:ARG:HG2   | 2.04                     | 0.58              |
| 19:CS:44:MET:N    | 19:CS:44:MET:SD    | 2.77                     | 0.58              |
| 19:CS:63:THR:HG22 | 19:CS:66:MET:CE    | 2.34                     | 0.58              |
| 55:D6:51:GLU:O    | 55:D6:52:VAL:CB    | 2.51                     | 0.58              |
| 27:DA:1887:C:H2'  | 27:DA:1888:G:H5''  | 1.85                     | 0.58              |
| 27:DA:2835:A:N6   | 27:DA:2878:U:H3'   | 2.18                     | 0.58              |
| 27:DA:531:C:OP1   | 27:DA:561:G:N1     | 2.36                     | 0.58              |
| 27:DA:696:G:C2    | 27:DA:767:U:O2     | 2.56                     | 0.58              |
| 27:DA:783:A:H2'   | 27:DA:784:A:C4'    | 2.32                     | 0.58              |
| 27:DA:848:G:H5'   | 27:DA:848:G:C8     | 2.39                     | 0.58              |
| 29:DC:194:ARG:C   | 29:DC:196:LEU:H    | 2.07                     | 0.58              |
| 32:DF:32:LEU:CD1  | 32:DF:112:MET:HE1  | 2.30                     | 0.58              |
| 33:DG:32:PRO:HB3  | 33:DG:172:LEU:HD22 | 1.84                     | 0.58              |
| 41:DS:87:PHE:HB2  | 41:DS:106:ARG:HH12 | 1.67                     | 0.58              |
| 27:DA:996:A:O2'   | 43:DU:92:ARG:HB3   | 2.03                     | 0.58              |
| 45:DW:92:ARG:O    | 45:DW:93:ALA:HB3   | 2.04                     | 0.58              |
| 1:AA:1015:A:H2'   | 1:AA:1016:A:C8     | 2.39                     | 0.58              |
| 1:AA:1059:C:O3'   | 14:AN:45:ARG:NH2   | 2.36                     | 0.58              |
| 1:AA:1220:G:H2'   | 1:AA:1221:G:C8     | 2.34                     | 0.58              |
| 1:AA:275:G:O2'    | 1:AA:276:G:H5'     | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:457:C:H2'    | 1:AA:458:C:H6     | 1.69                     | 0.58              |
| 1:AA:636:U:O2'    | 1:AA:637:G:H5'    | 2.03                     | 0.58              |
| 1:AA:19:C:H1'     | 1:AA:864:A:H1'    | 1.85                     | 0.58              |
| 2:AB:18:GLY:H     | 2:AB:42:ILE:CG2   | 2.07                     | 0.58              |
| 3:AC:83:ARG:O     | 3:AC:87:LEU:HG    | 2.04                     | 0.58              |
| 4:AD:170:VAL:CG1  | 4:AD:171:GLY:H    | 2.16                     | 0.58              |
| 13:AM:83:ASP:C    | 13:AM:85:GLY:N    | 2.55                     | 0.58              |
| 14:AN:26:ARG:NH2  | 14:AN:47:LEU:HD21 | 2.18                     | 0.58              |
| 16:AP:21:VAL:HG21 | 16:AP:59:TRP:CD2  | 2.39                     | 0.58              |
| 19:AS:11:VAL:HG22 | 19:AS:16:LEU:HD11 | 1.86                     | 0.58              |
| 24:AX:59:A:O2'    | 24:AX:60:U:O5'    | 2.21                     | 0.58              |
| 54:B5:56:LYS:H    | 54:B5:56:LYS:CD   | 2.12                     | 0.58              |
| 55:B6:41:PRO:CD   | 55:B6:46:HIS:CA   | 2.82                     | 0.58              |
| 55:B6:48:VAL:O    | 55:B6:49:HIS:HB2  | 2.03                     | 0.58              |
| 57:B8:10:ALA:O    | 57:B8:12:LYS:N    | 2.37                     | 0.58              |
| 58:B9:20:HIS:N    | 58:B9:20:HIS:ND1  | 2.51                     | 0.58              |
| 27:BA:1227:G:OP1  | 43:BU:13:LYS:HE3  | 2.03                     | 0.58              |
| 27:BA:1499:C:O2   | 27:BA:1499:C:H2'  | 2.03                     | 0.58              |
| 27:BA:2695:C:H2'  | 27:BA:2696:U:H6   | 1.68                     | 0.58              |
| 27:BA:2829:C:H2'  | 27:BA:2830:G:H8   | 1.69                     | 0.58              |
| 27:BA:2869:G:H2'  | 27:BA:2870:C:C6   | 2.39                     | 0.58              |
| 27:BA:74:A:H4'    | 27:BA:75:G:O5'    | 2.03                     | 0.58              |
| 30:BD:36:PRO:HB2  | 30:BD:61:LEU:CD1  | 2.34                     | 0.58              |
| 31:BE:4:ILE:HG22  | 31:BE:198:VAL:O   | 2.04                     | 0.58              |
| 35:BI:31:LEU:HD12 | 35:BI:31:LEU:N    | 2.19                     | 0.58              |
| 35:BI:16:GLY:HA2  | 35:BI:47:LEU:HD11 | 1.86                     | 0.58              |
| 37:BO:64:ARG:NH1  | 37:BO:81:ASP:OD2  | 2.36                     | 0.58              |
| 40:BR:76:VAL:HG12 | 40:BR:77:ARG:H    | 1.68                     | 0.58              |
| 40:BR:8:ARG:NE    | 40:BR:8:ARG:HA    | 2.18                     | 0.58              |
| 43:BU:31:SER:HG   | 43:BU:34:LYS:H    | 1.51                     | 0.58              |
| 46:BX:27:THR:HB   | 46:BX:80:ILE:HB   | 1.85                     | 0.58              |
| 47:BY:14:LEU:HD12 | 47:BY:15:VAL:H    | 1.69                     | 0.58              |
| 1:CA:1046:A:H3'   | 1:CA:1047:G:C8    | 2.39                     | 0.58              |
| 1:CA:107:G:C2'    | 1:CA:108:G:H5'    | 2.33                     | 0.58              |
| 1:CA:1500:A:OP2   | 1:CA:1505:G:OP1   | 2.22                     | 0.58              |
| 1:CA:419:C:H42    | 1:CA:424:G:H1     | 1.48                     | 0.58              |
| 1:CA:442:C:C5     | 1:CA:443:C:H5     | 2.22                     | 0.58              |
| 1:CA:542:G:OP1    | 4:CD:10:ARG:NH2   | 2.37                     | 0.58              |
| 1:CA:677:U:H3     | 1:CA:714:G:N2     | 1.99                     | 0.58              |
| 1:CA:994:A:H2     | 14:CN:4:LYS:HG3   | 1.68                     | 0.58              |
| 6:CF:4:TYR:N      | 6:CF:65:VAL:O     | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CH:10:LEU:HD13  | 8:CH:85:ARG:HG2   | 1.85                     | 0.58              |
| 12:CL:32:GLY:HA3  | 12:CL:57:LEU:HD13 | 1.85                     | 0.58              |
| 49:D0:20:ARG:NH1  | 49:D0:20:ARG:CG   | 2.58                     | 0.58              |
| 27:DA:2466:C:OP1  | 58:D9:4:ARG:HB2   | 2.03                     | 0.58              |
| 27:DA:1155:A:C5   | 27:DA:1157:G:N7   | 2.72                     | 0.58              |
| 27:DA:1876:A:H2'  | 27:DA:1877:A:C8   | 2.39                     | 0.58              |
| 27:DA:2725:A:O2'  | 27:DA:2726:U:O5'  | 2.22                     | 0.58              |
| 27:DA:693:C:O2'   | 27:DA:694:U:H5'   | 2.03                     | 0.58              |
| 27:DA:731:C:O2    | 27:DA:731:C:H2'   | 2.03                     | 0.58              |
| 27:DA:789:A:O3'   | 27:DA:1781:C:N4   | 2.37                     | 0.58              |
| 27:DA:803:U:O2'   | 27:DA:804:A:H5'   | 2.04                     | 0.58              |
| 30:DD:75:ILE:O    | 30:DD:76:PRO:O    | 2.21                     | 0.58              |
| 31:DE:110:GLY:HA2 | 31:DE:162:ALA:N   | 2.19                     | 0.58              |
| 31:DE:59:VAL:HG21 | 31:DE:63:LEU:HG   | 1.85                     | 0.58              |
| 32:DF:143:ALA:O   | 32:DF:146:ALA:HB3 | 2.03                     | 0.58              |
| 33:DG:109:VAL:O   | 33:DG:112:PRO:HB2 | 2.02                     | 0.58              |
| 33:DG:62:LEU:O    | 33:DG:143:GLU:HG3 | 2.04                     | 0.58              |
| 36:DN:51:PHE:CZ   | 36:DN:119:ARG:HD2 | 2.38                     | 0.58              |
| 36:DN:89:LYS:HB3  | 36:DN:89:LYS:NZ   | 2.17                     | 0.58              |
| 27:DA:662:G:C5'   | 38:DP:18:ARG:HA   | 2.32                     | 0.58              |
| 41:DS:90:GLY:C    | 41:DS:92:TYR:N    | 2.57                     | 0.58              |
| 42:DT:67:SER:O    | 42:DT:68:TYR:HB2  | 2.02                     | 0.58              |
| 48:DZ:75:LEU:HD13 | 48:DZ:82:PRO:CA   | 2.33                     | 0.58              |
| 1:AA:1004:A:H5''  | 1:AA:1025:U:N3    | 2.15                     | 0.58              |
| 1:AA:1085:U:C4'   | 1:AA:1086:U:OP2   | 2.52                     | 0.58              |
| 1:AA:1225:A:H5''  | 13:AM:103:THR:CG2 | 2.34                     | 0.58              |
| 2:AB:83:MET:HA    | 2:AB:83:MET:CE    | 2.33                     | 0.58              |
| 4:AD:153:ARG:CZ   | 4:AD:181:MET:HG3  | 2.34                     | 0.58              |
| 8:AH:58:TYR:O     | 8:AH:59:LEU:HD23  | 2.04                     | 0.58              |
| 10:AJ:50:ILE:HD13 | 10:AJ:60:ARG:HD3  | 1.84                     | 0.58              |
| 10:AJ:90:LEU:H    | 10:AJ:91:PRO:HD3  | 1.68                     | 0.58              |
| 11:AK:44:SER:OG   | 11:AK:47:VAL:HG23 | 2.04                     | 0.58              |
| 49:B0:37:LEU:O    | 49:B0:38:VAL:HG23 | 2.03                     | 0.58              |
| 50:B1:19:GLN:HA   | 50:B1:19:GLN:HE21 | 1.69                     | 0.58              |
| 27:BA:850:C:O2'   | 52:B3:46:ASN:ND2  | 2.37                     | 0.58              |
| 27:BA:2357:U:O2'  | 27:BA:2358:G:H5'' | 2.04                     | 0.58              |
| 27:BA:2591:C:H2'  | 27:BA:2592:G:C8   | 2.39                     | 0.58              |
| 29:BC:169:GLY:O   | 29:BC:171:ILE:N   | 2.37                     | 0.58              |
| 30:BD:10:THR:HG23 | 30:BD:13:ARG:HB3  | 1.84                     | 0.58              |
| 30:BD:149:PRO:O   | 30:BD:150:LYS:HB2 | 2.02                     | 0.58              |
| 31:BE:78:LEU:CD2  | 31:BE:78:LEU:N    | 2.61                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:BF:68:LYS:O    | 32:BF:70:THR:N    | 2.35                     | 0.58              |
| 34:BH:109:PHE:HE1 | 34:BH:152:ARG:CZ  | 2.16                     | 0.58              |
| 36:BN:58:ASP:O    | 36:BN:59:LYS:CB   | 2.50                     | 0.58              |
| 37:BO:105:GLU:HA  | 37:BO:108:GLU:OE2 | 2.03                     | 0.58              |
| 38:BP:29:LYS:HD2  | 38:BP:29:LYS:N    | 2.19                     | 0.58              |
| 38:BP:7:ARG:O     | 38:BP:10:PRO:HD2  | 2.04                     | 0.58              |
| 40:BR:99:LYS:HZ1  | 54:B5:43:HIS:HB3  | 1.69                     | 0.58              |
| 41:BS:56:LEU:HD22 | 41:BS:58:LEU:CD1  | 2.34                     | 0.58              |
| 43:BU:69:CYS:O    | 43:BU:74:LEU:CD1  | 2.52                     | 0.58              |
| 43:BU:8:VAL:CG1   | 43:BU:12:ARG:NE   | 2.65                     | 0.58              |
| 44:BV:19:LYS:HE2  | 44:BV:19:LYS:HA   | 1.86                     | 0.58              |
| 1:CA:538:G:H4'    | 12:CL:111:LYS:HD3 | 1.86                     | 0.58              |
| 1:CA:873:A:H4'    | 1:CA:874:G:OP2    | 2.03                     | 0.58              |
| 2:CB:96:ARG:N     | 2:CB:96:ARG:HD2   | 2.06                     | 0.58              |
| 3:CC:84:ILE:HD11  | 3:CC:101:LEU:HD22 | 1.84                     | 0.58              |
| 4:CD:199:ASN:O    | 4:CD:200:GLU:C    | 2.41                     | 0.58              |
| 9:CI:26:VAL:HG13  | 9:CI:61:ALA:O     | 2.03                     | 0.58              |
| 1:CA:1254:C:H41   | 10:CJ:43:ARG:NH1  | 2.01                     | 0.58              |
| 13:CM:10:PRO:CG   | 13:CM:18:ALA:HB1  | 2.34                     | 0.58              |
| 46:DX:5:TYR:CD2   | 51:D2:30:ARG:HA   | 2.39                     | 0.58              |
| 27:DA:1493:C:O2   | 27:DA:1493:C:C2'  | 2.51                     | 0.58              |
| 27:DA:1589:C:O2'  | 27:DA:1590:U:H5'  | 2.03                     | 0.58              |
| 27:DA:1669:A:C2   | 27:DA:1994:C:H1'  | 2.39                     | 0.58              |
| 27:DA:1965:C:H2'  | 27:DA:1966:A:C8   | 2.39                     | 0.58              |
| 27:DA:19:C:N4     | 27:DA:521:G:H1    | 2.01                     | 0.58              |
| 27:DA:2001:A:H2'  | 27:DA:2002:G:C8   | 2.38                     | 0.58              |
| 27:DA:2236:C:O2'  | 27:DA:2237:G:H5'  | 2.04                     | 0.58              |
| 27:DA:240:G:H3'   | 27:DA:241:A:H8    | 1.69                     | 0.58              |
| 27:DA:2416:C:H2'  | 27:DA:2417:C:C6   | 2.38                     | 0.58              |
| 27:DA:2478:A:H5'  | 58:D9:31:LYS:NZ   | 2.18                     | 0.58              |
| 27:DA:706:A:H2'   | 27:DA:707:G:O5'   | 2.04                     | 0.58              |
| 27:DA:729:G:C8    | 30:DD:208:LYS:HE2 | 2.39                     | 0.58              |
| 30:DD:226:MET:HB3 | 30:DD:230:ASP:HB2 | 1.84                     | 0.58              |
| 30:DD:69:ARG:HD2  | 30:DD:130:ALA:CB  | 2.34                     | 0.58              |
| 30:DD:70:TRP:O    | 30:DD:73:VAL:HG22 | 2.03                     | 0.58              |
| 31:DE:89:ASP:O    | 31:DE:90:THR:HB   | 2.03                     | 0.58              |
| 36:DN:132:ALA:O   | 36:DN:133:GLN:HB3 | 2.04                     | 0.58              |
| 39:DQ:121:ALA:O   | 39:DQ:125:LEU:HG  | 2.03                     | 0.58              |
| 40:DR:23:ASN:N    | 40:DR:23:ASN:HD22 | 2.02                     | 0.58              |
| 42:DT:16:ARG:CB   | 42:DT:19:LEU:HD11 | 2.34                     | 0.58              |
| 1:AA:424:G:H2'    | 1:AA:425:G:H8     | 1.69                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:187:LEU:HD13 | 2:AB:187:LEU:O     | 2.04                     | 0.58              |
| 2:AB:9:GLU:HA     | 2:AB:12:GLU:OE1    | 2.04                     | 0.58              |
| 3:AC:129:ALA:HB3  | 3:AC:132:ARG:CB    | 2.32                     | 0.58              |
| 1:AA:1255:G:H5''  | 3:AC:26:LYS:NZ     | 2.18                     | 0.58              |
| 5:AE:12:LEU:HD13  | 5:AE:12:LEU:C      | 2.24                     | 0.58              |
| 9:AI:114:TYR:H    | 9:AI:114:TYR:HD2   | 1.52                     | 0.58              |
| 1:AA:1128:C:C5'   | 9:AI:16:ARG:HH12   | 2.15                     | 0.58              |
| 7:AG:16:LEU:HD13  | 9:AI:44:VAL:HG23   | 1.84                     | 0.58              |
| 12:AL:25:LYS:CB   | 12:AL:30:ARG:HH12  | 2.17                     | 0.58              |
| 17:AQ:29:HIS:CE1  | 17:AQ:32:TYR:H     | 2.20                     | 0.58              |
| 20:AT:71:THR:CG2  | 20:AT:72:LEU:H     | 1.97                     | 0.58              |
| 54:B5:56:LYS:HG3  | 54:B5:59:GLU:HG3   | 1.86                     | 0.58              |
| 27:BA:1296:G:C2'  | 27:BA:1297:C:H5'   | 2.34                     | 0.58              |
| 27:BA:1321:A:H2'  | 27:BA:1322:A:H8    | 1.67                     | 0.58              |
| 27:BA:1762:A:C8   | 27:BA:1762:A:O5'   | 2.57                     | 0.58              |
| 27:BA:1771:C:O2'  | 27:BA:1786:A:C8    | 2.49                     | 0.58              |
| 27:BA:1891:G:H2'  | 27:BA:1892:C:H6    | 1.69                     | 0.58              |
| 27:BA:2081:C:O2'  | 27:BA:2082:A:H5'   | 2.03                     | 0.58              |
| 27:BA:413:C:O5'   | 27:BA:413:C:H6     | 1.87                     | 0.58              |
| 27:BA:459:U:H2'   | 27:BA:460:A:H8     | 1.69                     | 0.58              |
| 27:BA:620:G:H4'   | 27:BA:621:A:OP1    | 2.04                     | 0.58              |
| 28:BB:73:A:C4     | 28:BB:105:A:C2     | 2.92                     | 0.58              |
| 30:BD:118:VAL:CG2 | 30:BD:119:ALA:H    | 2.04                     | 0.58              |
| 32:BF:110:LEU:O   | 32:BF:110:LEU:HD13 | 2.03                     | 0.58              |
| 32:BF:40:GLN:OE1  | 32:BF:182:ASN:HB2  | 2.04                     | 0.58              |
| 35:BI:24:GLY:O    | 35:BI:25:TYR:C     | 2.41                     | 0.58              |
| 36:BN:113:GLY:HA2 | 36:BN:116:LEU:HD12 | 1.86                     | 0.58              |
| 37:BO:13:ASN:HD21 | 37:BO:96:THR:N     | 2.01                     | 0.58              |
| 38:BP:148:LEU:O   | 38:BP:149:GLU:HB2  | 2.03                     | 0.58              |
| 38:BP:23:PRO:CB   | 38:BP:33:ARG:HG3   | 2.30                     | 0.58              |
| 38:BP:62:LEU:HD23 | 38:BP:62:LEU:H     | 1.68                     | 0.58              |
| 38:BP:71:VAL:CG1  | 38:BP:72:PRO:CD    | 2.81                     | 0.58              |
| 40:BR:101:ALA:HB2 | 54:B5:44:THR:HB    | 1.86                     | 0.58              |
| 47:BY:14:LEU:HD23 | 47:BY:73:ARG:HD3   | 1.86                     | 0.58              |
| 1:CA:104:G:O2'    | 1:CA:105:G:H5'     | 2.04                     | 0.58              |
| 1:CA:1058:G:H2'   | 1:CA:1059:C:H6     | 1.66                     | 0.58              |
| 1:CA:808:C:O2'    | 1:CA:809:G:H5'     | 2.04                     | 0.58              |
| 5:CE:51:VAL:O     | 5:CE:55:VAL:HG23   | 2.03                     | 0.58              |
| 10:CJ:61:GLU:HG2  | 14:CN:58:LYS:HZ3   | 1.69                     | 0.58              |
| 13:CM:54:VAL:O    | 13:CM:58:GLU:HG2   | 2.03                     | 0.58              |
| 13:CM:70:LEU:O    | 13:CM:73:GLU:HB3   | 2.03                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1002:G:H8    | 27:DA:1002:G:O5'   | 1.87                     | 0.58              |
| 27:DA:1391:U:H2'   | 27:DA:1393:A:OP2   | 2.04                     | 0.58              |
| 27:DA:1462:C:H2'   | 27:DA:1463:C:H6    | 1.69                     | 0.58              |
| 27:DA:2171:A:H4'   | 27:DA:2172:U:OP1   | 2.03                     | 0.58              |
| 27:DA:2235:G:H2'   | 27:DA:2236:C:C6    | 2.39                     | 0.58              |
| 27:DA:2415:G:H2'   | 27:DA:2416:C:C6    | 2.38                     | 0.58              |
| 27:DA:397:G:O2'    | 27:DA:398:G:H5'    | 2.04                     | 0.58              |
| 29:DC:168:THR:HA   | 29:DC:173:ALA:HB2  | 1.86                     | 0.58              |
| 33:DG:6:ALA:HB3    | 33:DG:104:GLU:CD   | 2.24                     | 0.58              |
| 33:DG:98:ARG:HA    | 33:DG:101:ILE:HG23 | 1.85                     | 0.58              |
| 27:DA:2746:U:H1'   | 34:DH:139:GLN:CB   | 2.33                     | 0.58              |
| 27:DA:245:G:C5'    | 38:DP:69:GLY:HA3   | 2.34                     | 0.58              |
| 41:DS:42:ASP:O     | 41:DS:43:GLU:C     | 2.41                     | 0.58              |
| 42:DT:1:MET:C      | 42:DT:3:ARG:H      | 2.05                     | 0.58              |
| 27:DA:1336:A:OP1   | 46:DX:64:LYS:HE3   | 2.04                     | 0.58              |
| 47:DY:14:LEU:HD12  | 47:DY:15:VAL:H     | 1.69                     | 0.58              |
| 1:AA:413:G:N2      | 1:AA:428:G:H1'     | 2.19                     | 0.57              |
| 1:AA:544:G:OP1     | 4:AD:59:ARG:NH2    | 2.36                     | 0.57              |
| 1:AA:657:G:C2      | 1:AA:658:G:C8      | 2.92                     | 0.57              |
| 1:AA:728:A:C6      | 15:AO:54:ARG:HD2   | 2.38                     | 0.57              |
| 1:AA:96:U:H2'      | 1:AA:97:G:H8       | 1.68                     | 0.57              |
| 12:AL:38:ARG:CG    | 12:AL:39:THR:H     | 2.09                     | 0.57              |
| 16:AP:21:VAL:HG13  | 16:AP:33:ILE:CB    | 2.30                     | 0.57              |
| 24:AX:17:C:O2      | 24:AX:17(B):U:H5   | 1.87                     | 0.57              |
| 7:AG:86:GLN:HE22   | 25:AY:30:A:H2      | 1.49                     | 0.57              |
| 25:AY:64:G:O2'     | 25:AY:65:U:H5'     | 2.04                     | 0.57              |
| 55:B6:19:ARG:HB2   | 55:B6:21:TYR:OH    | 2.04                     | 0.57              |
| 27:BA:1051:G:O2'   | 27:BA:1052:C:C6    | 2.56                     | 0.57              |
| 27:BA:1652:A:O2'   | 27:BA:1653:G:H5'   | 2.04                     | 0.57              |
| 27:BA:1711:C:H2'   | 27:BA:1712:C:C6    | 2.39                     | 0.57              |
| 27:BA:1779:U:C5    | 27:BA:1784:A:N7    | 2.72                     | 0.57              |
| 27:BA:182:A:C2     | 27:BA:183:C:C2     | 2.92                     | 0.57              |
| 27:BA:1848:A:C2'   | 27:BA:1849:G:H8    | 2.16                     | 0.57              |
| 27:BA:1926:U:H2'   | 27:BA:1928:A:OP2   | 2.03                     | 0.57              |
| 27:BA:2394:C:OP1   | 38:BP:63:PRO:HD2   | 2.04                     | 0.57              |
| 27:BA:2648:C:H2'   | 27:BA:2649:U:C6    | 2.39                     | 0.57              |
| 27:BA:2681:C:H5    | 27:BA:2725:A:N6    | 2.00                     | 0.57              |
| 13:AM:94:ARG:NH1   | 27:BA:887:A:H5''   | 2.18                     | 0.57              |
| 31:BE:167:VAL:CG2  | 31:BE:170:LEU:HD11 | 2.33                     | 0.57              |
| 36:BN:112:LEU:HD12 | 36:BN:112:LEU:O    | 2.04                     | 0.57              |
| 38:BP:23:PRO:HB2   | 38:BP:33:ARG:HD2   | 1.84                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BP:62:LEU:HB2   | 38:BP:63:PRO:HD2   | 1.86                     | 0.57              |
| 41:BS:90:GLY:C     | 41:BS:92:TYR:H     | 2.07                     | 0.57              |
| 42:BT:31:SER:C     | 42:BT:32:TYR:CD2   | 2.77                     | 0.57              |
| 48:BZ:157:PRO:HG2  | 48:BZ:160:VAL:CG2  | 2.31                     | 0.57              |
| 39:BQ:141:GLN:HG3  | 48:BZ:71:ARG:NH1   | 2.19                     | 0.57              |
| 1:CA:1496:C:H2'    | 1:CA:1497:G:O4'    | 2.04                     | 0.57              |
| 1:CA:177:C:H2'     | 1:CA:178:C:H6      | 1.69                     | 0.57              |
| 1:CA:279:A:O2'     | 1:CA:280:C:OP2     | 2.17                     | 0.57              |
| 1:CA:509:A:H4'     | 1:CA:510:A:OP1     | 2.03                     | 0.57              |
| 1:CA:825:G:H22     | 8:CH:11:THR:HG21   | 1.69                     | 0.57              |
| 1:CA:980:C:O2      | 1:CA:980:C:H2'     | 2.02                     | 0.57              |
| 2:CB:132:LYS:HA    | 2:CB:135:GLN:HB2   | 1.84                     | 0.57              |
| 1:CA:546:G:OP1     | 4:CD:72:GLU:HB3    | 2.04                     | 0.57              |
| 12:CL:72:HIS:CD2   | 12:CL:74:LEU:HB2   | 2.39                     | 0.57              |
| 16:CP:45:THR:C     | 16:CP:47:ASP:H     | 2.07                     | 0.57              |
| 17:CQ:29:HIS:CG    | 17:CQ:30:PRO:HD2   | 2.39                     | 0.57              |
| 1:CA:1286:A:C2     | 21:CU:22:ARG:NH2   | 2.71                     | 0.57              |
| 23:CW:51:G:H1      | 23:CW:61:C:H42     | 1.51                     | 0.57              |
| 24:CX:23:C:H2'     | 24:CX:24:U:C6      | 2.38                     | 0.57              |
| 55:D6:52:VAL:O     | 55:D6:52:VAL:HG12  | 2.02                     | 0.57              |
| 27:DA:146:G:C6     | 27:DA:147:U:C4     | 2.91                     | 0.57              |
| 27:DA:1889:A:H1'   | 27:DA:2087:G:H5'   | 1.85                     | 0.57              |
| 27:DA:1943:U:H4'   | 27:DA:1944:U:O5'   | 2.03                     | 0.57              |
| 27:DA:2103:C:C3'   | 27:DA:2104:G:H5''  | 2.33                     | 0.57              |
| 27:DA:2195:C:C2'   | 27:DA:2196:C:H5'   | 2.33                     | 0.57              |
| 27:DA:2850:A:OP2   | 27:DA:2866:U:C5    | 2.57                     | 0.57              |
| 27:DA:612:C:N4     | 27:DA:615:G:H1     | 2.02                     | 0.57              |
| 29:DC:44:HIS:O     | 29:DC:210:ARG:HA   | 2.04                     | 0.57              |
| 32:DF:186:ILE:HG23 | 32:DF:192:LEU:CD1  | 2.32                     | 0.57              |
| 33:DG:21:ARG:HD3   | 33:DG:22:ARG:N     | 2.19                     | 0.57              |
| 34:DH:105:LEU:HD23 | 34:DH:115:VAL:HG21 | 1.86                     | 0.57              |
| 35:DI:51:ILE:HG22  | 35:DI:52:ARG:N     | 2.18                     | 0.57              |
| 36:DN:108:PRO:O    | 36:DN:113:GLY:HA3  | 2.04                     | 0.57              |
| 36:DN:133:GLN:HG2  | 36:DN:134:ARG:N    | 2.17                     | 0.57              |
| 42:DT:102:ILE:HD12 | 42:DT:110:ILE:HD11 | 1.84                     | 0.57              |
| 43:DU:102:GLU:OE1  | 44:DV:2:PHE:HE1    | 1.87                     | 0.57              |
| 44:DV:61:VAL:C     | 44:DV:62:LEU:HD13  | 2.23                     | 0.57              |
| 47:DY:31:LEU:HB2   | 47:DY:32:PRO:HA    | 1.85                     | 0.57              |
| 47:DY:88:LYS:NZ    | 47:DY:93:GLY:HA3   | 2.19                     | 0.57              |
| 1:AA:1087:G:H2'    | 1:AA:1088:G:C8     | 2.39                     | 0.57              |
| 1:AA:1202:G:H2'    | 1:AA:1203:C:O4'    | 2.04                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1263:C:C2'   | 1:AA:1264:C:H5'    | 2.34                     | 0.57              |
| 1:AA:528:C:H5'    | 1:AA:535:A:N1      | 2.19                     | 0.57              |
| 1:AA:705:U:C5     | 1:AA:706:A:C5      | 2.92                     | 0.57              |
| 1:AA:876:G:H2'    | 1:AA:877:C:H6      | 1.68                     | 0.57              |
| 3:AC:68:VAL:HG12  | 3:AC:70:VAL:HG23   | 1.85                     | 0.57              |
| 3:AC:90:GLU:HA    | 3:AC:93:LYS:HB2    | 1.86                     | 0.57              |
| 3:AC:90:GLU:O     | 3:AC:93:LYS:HB2    | 2.04                     | 0.57              |
| 14:AN:24:CYS:HB3  | 14:AN:27:CYS:O     | 2.05                     | 0.57              |
| 18:AR:44:LEU:HD13 | 18:AR:48:GLY:O     | 2.04                     | 0.57              |
| 23:AW:4:G:H2'     | 23:AW:5:G:H5'      | 1.85                     | 0.57              |
| 24:AX:39:C:H6     | 24:AX:39:C:O5'     | 1.87                     | 0.57              |
| 27:BA:1029:A:C2'  | 27:BA:1030:G:H5'   | 2.33                     | 0.57              |
| 27:BA:1556:C:H2'  | 27:BA:1557:C:H6    | 1.69                     | 0.57              |
| 27:BA:1956:U:H2'  | 27:BA:1957:C:C5'   | 2.32                     | 0.57              |
| 27:BA:2373:G:H2'  | 27:BA:2374:C:C6    | 2.39                     | 0.57              |
| 27:BA:2555:U:H2'  | 27:BA:2556:C:O4'   | 2.03                     | 0.57              |
| 27:BA:2787:C:O2'  | 31:BE:61:ARG:HB2   | 2.04                     | 0.57              |
| 27:BA:335:C:H2'   | 27:BA:336:C:C6     | 2.37                     | 0.57              |
| 27:BA:827:U:H2'   | 27:BA:2068:U:N3    | 2.18                     | 0.57              |
| 27:BA:84:A:H5'    | 47:BY:9:LYS:HB3    | 1.86                     | 0.57              |
| 29:BC:20:TYR:CG   | 29:BC:21:THR:N     | 2.71                     | 0.57              |
| 30:BD:154:LYS:C   | 30:BD:155:LEU:HD12 | 2.23                     | 0.57              |
| 35:BI:77:LEU:HB3  | 35:BI:140:LEU:CD1  | 2.32                     | 0.57              |
| 35:BI:8:PRO:O     | 35:BI:9:LEU:HD23   | 2.04                     | 0.57              |
| 38:BP:17:LYS:HG2  | 38:BP:17:LYS:O     | 2.03                     | 0.57              |
| 41:BS:15:ARG:O    | 41:BS:18:ILE:HG22  | 2.04                     | 0.57              |
| 44:BV:35:LEU:C    | 44:BV:37:VAL:N     | 2.55                     | 0.57              |
| 44:BV:64:HIS:HA   | 44:BV:92:THR:HA    | 1.86                     | 0.57              |
| 46:BX:26:TYR:HB3  | 46:BX:92:LEU:HD12  | 1.85                     | 0.57              |
| 47:BY:32:PRO:C    | 47:BY:34:LYS:H     | 2.08                     | 0.57              |
| 1:CA:1237:C:O2    | 1:CA:1334:G:O2'    | 2.14                     | 0.57              |
| 1:CA:41:G:O2'     | 1:CA:42:G:H5'      | 2.04                     | 0.57              |
| 1:CA:47:C:O2'     | 1:CA:48:C:H5'      | 2.04                     | 0.57              |
| 2:CB:32:ILE:HA    | 2:CB:42:ILE:HA     | 1.86                     | 0.57              |
| 3:CC:36:ASP:O     | 3:CC:40:ARG:NH1    | 2.37                     | 0.57              |
| 3:CC:73:PRO:C     | 3:CC:75:VAL:N      | 2.57                     | 0.57              |
| 5:CE:147:ASP:N    | 5:CE:147:ASP:OD2   | 2.35                     | 0.57              |
| 6:CF:86:ARG:O     | 6:CF:87:ARG:HG2    | 2.03                     | 0.57              |
| 9:CI:46:ALA:HB2   | 9:CI:74:ILE:HG23   | 1.86                     | 0.57              |
| 16:CP:74:LEU:O    | 16:CP:77:ALA:HB3   | 2.05                     | 0.57              |
| 20:CT:73:HIS:O    | 20:CT:76:ALA:HB3   | 2.03                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:CU:2:GLY:O     | 21:CU:4:GLY:N     | 2.37                     | 0.57              |
| 51:D2:50:ILE:O    | 51:D2:52:ASP:N    | 2.38                     | 0.57              |
| 57:D8:55:ALA:O    | 57:D8:58:ILE:HB   | 2.04                     | 0.57              |
| 27:DA:1010:A:O2'  | 27:DA:1011:G:H5'  | 2.04                     | 0.57              |
| 27:DA:1639:U:H2'  | 27:DA:1640:C:C5'  | 2.33                     | 0.57              |
| 27:DA:2239:G:H2'  | 27:DA:2240:C:O4'  | 2.05                     | 0.57              |
| 27:DA:2468:G:OP1  | 39:DQ:119:ARG:NH2 | 2.36                     | 0.57              |
| 27:DA:2520:C:H2'  | 27:DA:2521:C:C6   | 2.40                     | 0.57              |
| 27:DA:2536:G:O2'  | 27:DA:2537:U:H5'  | 2.04                     | 0.57              |
| 27:DA:2545:G:N2   | 27:DA:2546:U:H1'  | 2.18                     | 0.57              |
| 27:DA:2593:U:C2   | 27:DA:2594:C:C5   | 2.92                     | 0.57              |
| 27:DA:2734:A:H62  | 27:DA:2770:G:N2   | 2.00                     | 0.57              |
| 27:DA:2745:C:H5'  | 34:DH:146:ALA:HB2 | 1.85                     | 0.57              |
| 27:DA:2840:C:H2'  | 27:DA:2841:C:C6   | 2.39                     | 0.57              |
| 27:DA:2876:G:N2   | 27:DA:2877:G:H1'  | 2.19                     | 0.57              |
| 27:DA:7:G:H1      | 27:DA:2896:C:N4   | 2.01                     | 0.57              |
| 27:DA:463:G:N2    | 27:DA:466:A:OP2   | 2.34                     | 0.57              |
| 27:DA:482:A:H62   | 27:DA:506:G:C2'   | 2.17                     | 0.57              |
| 27:DA:589:C:H2'   | 27:DA:590:A:C8    | 2.39                     | 0.57              |
| 27:DA:740:U:H6    | 27:DA:740:U:C5'   | 2.09                     | 0.57              |
| 27:DA:862:G:C2    | 27:DA:863:A:H1'   | 2.38                     | 0.57              |
| 27:DA:865:C:C2'   | 27:DA:865:C:O2    | 2.51                     | 0.57              |
| 28:DB:43:C:H5'    | 28:DB:44:G:OP2    | 2.04                     | 0.57              |
| 32:DF:20:LEU:HB3  | 32:DF:23:ASP:OD1  | 2.05                     | 0.57              |
| 35:DI:7:GLU:CG    | 35:DI:8:PRO:HD2   | 2.34                     | 0.57              |
| 38:DP:108:LYS:HD2 | 38:DP:108:LYS:N   | 2.18                     | 0.57              |
| 27:DA:587:C:H3'   | 38:DP:33:ARG:HH22 | 1.68                     | 0.57              |
| 38:DP:64:LYS:HB3  | 57:D8:25:MET:HG3  | 1.85                     | 0.57              |
| 27:DA:1275:A:C8   | 40:DR:16:HIS:CD2  | 2.92                     | 0.57              |
| 42:DT:23:ARG:NH2  | 42:DT:120:ARG:HD3 | 2.19                     | 0.57              |
| 45:DW:11:ARG:C    | 45:DW:11:ARG:HE   | 2.07                     | 0.57              |
| 47:DY:19:LYS:HG2  | 47:DY:19:LYS:O    | 2.05                     | 0.57              |
| 47:DY:47:LYS:HD2  | 47:DY:47:LYS:N    | 2.19                     | 0.57              |
| 47:DY:49:VAL:O    | 47:DY:53:PRO:HG3  | 2.04                     | 0.57              |
| 48:DZ:94:PRO:HB2  | 48:DZ:126:LYS:HZ2 | 1.67                     | 0.57              |
| 1:AA:1293:G:H2'   | 1:AA:1294:G:H8    | 1.68                     | 0.57              |
| 1:AA:346:G:H5''   | 42:BT:41:ARG:HE   | 1.68                     | 0.57              |
| 1:AA:373:A:O2'    | 1:AA:451:A:N7     | 2.37                     | 0.57              |
| 1:AA:537:G:H2'    | 1:AA:538:G:H8     | 1.68                     | 0.57              |
| 1:AA:644:G:C2'    | 1:AA:645:C:H5'    | 2.33                     | 0.57              |
| 2:AB:103:THR:OG1  | 2:AB:176:GLU:HG3  | 2.04                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AC:145:GLY:O    | 3:AC:146:ALA:HB2   | 2.04                     | 0.57              |
| 6:AF:97:PHE:CZ    | 18:AR:61:LYS:HE2   | 2.40                     | 0.57              |
| 9:AI:112:LYS:HA   | 9:AI:119:ALA:H     | 1.69                     | 0.57              |
| 13:AM:22:ILE:HG21 | 13:AM:25:ILE:HD13  | 1.85                     | 0.57              |
| 17:AQ:57:VAL:HA   | 17:AQ:77:VAL:HG23  | 1.86                     | 0.57              |
| 23:AW:32:U:H2'    | 23:AW:34:U:H5      | 1.68                     | 0.57              |
| 23:AW:42:G:H2'    | 23:AW:43:C:H5''    | 1.85                     | 0.57              |
| 57:B8:7:HIS:HB2   | 57:B8:59:LYS:HB3   | 1.87                     | 0.57              |
| 27:BA:1459:G:N3   | 27:BA:1459:G:H2'   | 2.18                     | 0.57              |
| 27:BA:1627:G:C2   | 27:BA:1628:G:C8    | 2.91                     | 0.57              |
| 27:BA:1640:C:H2'  | 27:BA:1641:A:H5'   | 1.86                     | 0.57              |
| 27:BA:1991:U:H2'  | 27:BA:1992:G:H5''  | 1.85                     | 0.57              |
| 27:BA:2099:U:OP2  | 27:BA:2099:U:H6    | 1.86                     | 0.57              |
| 27:BA:2528:U:H2'  | 27:BA:2530:A:O5'   | 2.03                     | 0.57              |
| 27:BA:498:G:O2'   | 27:BA:499:U:H5'    | 2.04                     | 0.57              |
| 27:BA:924:C:O2'   | 27:BA:925:C:H5'    | 2.04                     | 0.57              |
| 30:BD:33:LEU:O    | 30:BD:34:VAL:CG1   | 2.47                     | 0.57              |
| 30:BD:34:VAL:O    | 30:BD:35:LYS:HD3   | 2.05                     | 0.57              |
| 30:BD:65:ILE:HA   | 30:BD:104:TYR:HB2  | 1.85                     | 0.57              |
| 27:BA:674:G:OP1   | 32:BF:76:GLY:HA3   | 2.05                     | 0.57              |
| 33:BG:53:LEU:N    | 33:BG:53:LEU:HD22  | 2.18                     | 0.57              |
| 42:BT:30:VAL:HG21 | 42:BT:83:ILE:HG13  | 1.85                     | 0.57              |
| 42:BT:91:ARG:CA   | 42:BT:116:ALA:HA   | 2.34                     | 0.57              |
| 45:BW:79:GLY:C    | 45:BW:100:THR:HG22 | 2.24                     | 0.57              |
| 1:CA:1209:C:O2'   | 1:CA:1210:C:H5'    | 2.03                     | 0.57              |
| 1:CA:1321:C:C3'   | 1:CA:1322:C:H5''   | 2.35                     | 0.57              |
| 1:CA:1409:C:H2'   | 1:CA:1410:G:C8     | 2.40                     | 0.57              |
| 1:CA:648:A:H2'    | 1:CA:649:G:C8      | 2.39                     | 0.57              |
| 1:CA:990:C:H2'    | 1:CA:991:U:C6      | 2.38                     | 0.57              |
| 3:CC:150:LYS:HG3  | 3:CC:169:ALA:HB2   | 1.86                     | 0.57              |
| 7:CG:32:ARG:O     | 7:CG:33:ASP:HB2    | 2.03                     | 0.57              |
| 8:CH:82:HIS:HE2   | 8:CH:136:GLU:CD    | 2.07                     | 0.57              |
| 14:CN:23:ARG:NH1  | 14:CN:30:ALA:HB2   | 2.18                     | 0.57              |
| 20:CT:63:ILE:HD13 | 20:CT:80:ARG:CB    | 2.34                     | 0.57              |
| 49:D0:40:GLN:OE1  | 49:D0:45:PHE:HB2   | 2.04                     | 0.57              |
| 53:D4:46:ASN:HD22 | 53:D4:47:VAL:H     | 1.53                     | 0.57              |
| 56:D7:25:PRO:HG3  | 56:D7:28:ARG:NH2   | 2.19                     | 0.57              |
| 27:DA:1116:C:H2'  | 27:DA:1117:G:H8    | 1.69                     | 0.57              |
| 27:DA:1688:U:H3   | 27:DA:1700:A:C5'   | 2.17                     | 0.57              |
| 27:DA:1796:U:O2   | 27:DA:1824:G:C2    | 2.57                     | 0.57              |
| 27:DA:296:C:O2'   | 27:DA:297:C:H5'    | 2.03                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:414:C:H2'    | 27:DA:415:A:C8     | 2.36                     | 0.57              |
| 27:DA:628:G:C6     | 27:DA:636:G:C2     | 2.92                     | 0.57              |
| 27:DA:701:G:H1     | 27:DA:731:C:H42    | 1.53                     | 0.57              |
| 27:DA:992:C:O2'    | 27:DA:993:G:H5'    | 2.05                     | 0.57              |
| 30:DD:102:LYS:O    | 30:DD:103:ARG:HG2  | 2.04                     | 0.57              |
| 27:DA:2787:C:O2'   | 31:DE:61:ARG:HG3   | 2.05                     | 0.57              |
| 32:DF:103:LYS:HA   | 32:DF:106:ARG:HG3  | 1.85                     | 0.57              |
| 32:DF:28:ILE:O     | 32:DF:30:PRO:HD3   | 2.04                     | 0.57              |
| 36:DN:33:LEU:HG    | 36:DN:38:HIS:CE1   | 2.39                     | 0.57              |
| 42:DT:126:ALA:C    | 42:DT:128:GLU:H    | 2.07                     | 0.57              |
| 43:DU:69:CYS:O     | 43:DU:72:HIS:HB2   | 2.04                     | 0.57              |
| 1:AA:11:G:C5       | 1:AA:12:U:C5       | 2.92                     | 0.57              |
| 1:AA:443:C:H2'     | 1:AA:444:C:H6      | 1.68                     | 0.57              |
| 1:AA:979:C:H42     | 14:AN:18:VAL:HG12  | 1.70                     | 0.57              |
| 2:AB:151:GLY:O     | 2:AB:152:PHE:CB    | 2.52                     | 0.57              |
| 3:AC:134:ILE:HG23  | 3:AC:151:VAL:HG12  | 1.86                     | 0.57              |
| 1:AA:430:A:P       | 4:AD:8:VAL:H       | 2.27                     | 0.57              |
| 5:AE:129:ILE:CG2   | 5:AE:130:ASN:N     | 2.54                     | 0.57              |
| 7:AG:71:PRO:HA     | 7:AG:138:LYS:HG3   | 1.87                     | 0.57              |
| 11:AK:111:ASP:HA   | 18:AR:84:LYS:HG3   | 1.87                     | 0.57              |
| 11:AK:39:PRO:C     | 11:AK:40:ILE:HD13  | 2.25                     | 0.57              |
| 12:AL:15:VAL:CG2   | 12:AL:16:ARG:H     | 2.16                     | 0.57              |
| 14:AN:60:SER:O     | 14:AN:61:TRP:HB3   | 2.04                     | 0.57              |
| 25:AY:37:U:H2'     | 25:AY:38:U:C4'     | 2.34                     | 0.57              |
| 7:AG:148:ASN:ND2   | 25:AY:39:C:H4'     | 2.20                     | 0.57              |
| 50:B1:18:ILE:O     | 50:B1:19:GLN:NE2   | 2.35                     | 0.57              |
| 52:B3:26:LEU:O     | 52:B3:35:ARG:NE    | 2.34                     | 0.57              |
| 54:B5:52:TYR:O     | 54:B5:53:ALA:C     | 2.41                     | 0.57              |
| 27:BA:110:G:H2'    | 27:BA:111:A:H8     | 1.70                     | 0.57              |
| 27:BA:1204:A:O2'   | 27:BA:1205:U:OP2   | 2.17                     | 0.57              |
| 27:BA:2103:C:H42   | 27:BA:2186:G:H1    | 1.53                     | 0.57              |
| 27:BA:2311:A:H4'   | 27:BA:2312:U:OP1   | 2.04                     | 0.57              |
| 27:BA:363(F):A:O2' | 27:BA:364:C:C5     | 2.56                     | 0.57              |
| 27:BA:528:A:O5'    | 27:BA:528:A:C8     | 2.57                     | 0.57              |
| 27:BA:628:G:O2'    | 27:BA:629:G:O4'    | 2.19                     | 0.57              |
| 27:BA:736:C:O2'    | 27:BA:737:C:H5'    | 2.04                     | 0.57              |
| 30:BD:72:LYS:HZ3   | 30:BD:103:ARG:HH12 | 1.52                     | 0.57              |
| 30:BD:183:ARG:HG2  | 30:BD:183:ARG:HH11 | 1.69                     | 0.57              |
| 27:BA:2227:A:H5'   | 30:BD:263:ARG:HH11 | 1.69                     | 0.57              |
| 30:BD:49:ILE:CD1   | 30:BD:52:ARG:HA    | 2.26                     | 0.57              |
| 30:BD:66:ASP:OD2   | 30:BD:69:ARG:HG2   | 2.04                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:BG:111:LEU:HD22 | 33:BG:117:PHE:CE2 | 2.40                     | 0.57              |
| 33:BG:118:ARG:H    | 33:BG:181:ARG:NH2 | 1.97                     | 0.57              |
| 35:BI:30:LEU:HA    | 35:BI:35:LEU:HB2  | 1.87                     | 0.57              |
| 40:BR:18:LEU:CD1   | 40:BR:22:ARG:NE   | 2.67                     | 0.57              |
| 42:BT:28:VAL:O     | 42:BT:29:ARG:CG   | 2.53                     | 0.57              |
| 44:BV:6:LYS:HG3    | 44:BV:11:GLN:HG2  | 1.85                     | 0.57              |
| 44:BV:82:ARG:C     | 44:BV:83:ARG:HG2  | 2.25                     | 0.57              |
| 1:CA:181:G:H21     | 1:CA:183:G:H22    | 1.51                     | 0.57              |
| 1:CA:67:C:H2'      | 1:CA:68:G:H8      | 1.67                     | 0.57              |
| 1:CA:978:A:H8      | 1:CA:978:A:H5''   | 1.68                     | 0.57              |
| 2:CB:134:GLU:HA    | 2:CB:137:ARG:CB   | 2.34                     | 0.57              |
| 2:CB:32:ILE:HD11   | 2:CB:40:HIS:CB    | 2.25                     | 0.57              |
| 2:CB:82:ARG:HA     | 2:CB:92:TYR:CE2   | 2.39                     | 0.57              |
| 4:CD:102:ASP:HB3   | 4:CD:136:PRO:HA   | 1.86                     | 0.57              |
| 5:CE:96:PRO:HA     | 5:CE:117:ASP:OD2  | 2.05                     | 0.57              |
| 8:CH:6:ILE:HG22    | 8:CH:7:ALA:N      | 2.18                     | 0.57              |
| 9:CI:41:VAL:HG12   | 9:CI:41:VAL:O     | 2.04                     | 0.57              |
| 10:CJ:30:SER:OG    | 10:CJ:81:THR:HG22 | 2.04                     | 0.57              |
| 11:CK:65:ALA:HB1   | 11:CK:98:LEU:CD2  | 2.34                     | 0.57              |
| 11:CK:69:ALA:O     | 11:CK:73:MET:HG3  | 2.04                     | 0.57              |
| 11:CK:86:GLY:O     | 11:CK:87:THR:O    | 2.22                     | 0.57              |
| 14:CN:39:LEU:HD12  | 14:CN:44:LEU:HA   | 1.85                     | 0.57              |
| 15:CO:37:ASN:N     | 15:CO:37:ASN:ND2  | 2.53                     | 0.57              |
| 15:CO:85:LEU:HB3   | 15:CO:87:ILE:HD11 | 1.86                     | 0.57              |
| 16:CP:71:ARG:O     | 16:CP:74:LEU:HB2  | 2.04                     | 0.57              |
| 20:CT:88:VAL:HG12  | 20:CT:88:VAL:O    | 2.04                     | 0.57              |
| 26:CZ:3:SER:O      | 26:CZ:5:UAL:N     | 2.37                     | 0.57              |
| 54:D5:31:VAL:O     | 54:D5:39:MET:HB3  | 2.04                     | 0.57              |
| 27:DA:1229:G:O2'   | 27:DA:1230:C:H5'  | 2.03                     | 0.57              |
| 27:DA:141:A:C8     | 27:DA:1408:C:O2'  | 2.55                     | 0.57              |
| 27:DA:1490:A:H5'   | 27:DA:1494:A:H62  | 1.69                     | 0.57              |
| 27:DA:1893:C:C2'   | 27:DA:1894:C:O5'  | 2.53                     | 0.57              |
| 27:DA:1929:G:H4'   | 27:DA:1930:G:OP1  | 2.04                     | 0.57              |
| 27:DA:2682:U:H5'   | 27:DA:2682:U:C6   | 2.40                     | 0.57              |
| 27:DA:380:U:H2'    | 27:DA:381:G:H8    | 1.69                     | 0.57              |
| 27:DA:985:C:H2'    | 27:DA:986:C:C6    | 2.39                     | 0.57              |
| 30:DD:26:LYS:O     | 30:DD:27:THR:CB   | 2.51                     | 0.57              |
| 38:DP:87:ASP:C     | 38:DP:89:ALA:N    | 2.56                     | 0.57              |
| 40:DR:37:THR:OG1   | 40:DR:40:LYS:HB2  | 2.04                     | 0.57              |
| 42:DT:123:GLN:O    | 42:DT:126:ALA:HB3 | 2.03                     | 0.57              |
| 42:DT:29:ARG:HG3   | 42:DT:30:VAL:HG13 | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:DY:43:ASN:ND2  | 47:DY:64:GLU:HG3  | 2.19                     | 0.57              |
| 47:DY:4:LYS:HG3   | 47:DY:5:MET:N     | 2.20                     | 0.57              |
| 1:AA:1414:U:H3    | 1:AA:1486:G:H1    | 1.50                     | 0.57              |
| 1:AA:189(I):G:H2' | 1:AA:189(J):G:C8  | 2.40                     | 0.57              |
| 1:AA:730:G:C5     | 1:AA:731:G:H1'    | 2.39                     | 0.57              |
| 1:AA:743:U:O2'    | 1:AA:744:C:H5'    | 2.04                     | 0.57              |
| 3:AC:40:ARG:HB3   | 3:AC:44:GLU:OE2   | 2.04                     | 0.57              |
| 5:AE:20:GLN:HE22  | 5:AE:25:ARG:NH2   | 2.02                     | 0.57              |
| 13:AM:15:VAL:HG23 | 13:AM:16:ASP:N    | 2.18                     | 0.57              |
| 14:AN:9:LYS:HG3   | 14:AN:12:ARG:NH1  | 2.19                     | 0.57              |
| 57:B8:14:VAL:HG21 | 57:B8:22:VAL:HG12 | 1.86                     | 0.57              |
| 27:BA:185:U:H2'   | 27:BA:186:G:C8    | 2.38                     | 0.57              |
| 27:BA:2307:G:H3'  | 27:BA:2307:G:N3   | 2.20                     | 0.57              |
| 27:BA:2492:U:H2'  | 27:BA:2493:U:H6   | 1.70                     | 0.57              |
| 27:BA:425:G:O2'   | 27:BA:426:C:H5'   | 2.05                     | 0.57              |
| 27:BA:606:U:H4'   | 27:BA:658:C:H4'   | 1.86                     | 0.57              |
| 27:BA:99:U:O4'    | 27:BA:99:U:O2     | 2.22                     | 0.57              |
| 29:BC:41:VAL:CA   | 29:BC:213:TYR:HA  | 2.16                     | 0.57              |
| 30:BD:186:HIS:CD2 | 30:BD:188:GLU:HG2 | 2.39                     | 0.57              |
| 31:BE:113:PHE:HE2 | 31:BE:157:ALA:HB1 | 1.68                     | 0.57              |
| 31:BE:13:ARG:HD2  | 31:BE:20:ALA:HB1  | 1.85                     | 0.57              |
| 32:BF:22:ALA:HA   | 32:BF:26:ALA:HB2  | 1.85                     | 0.57              |
| 32:BF:45:ARG:NH1  | 32:BF:97:TYR:CD1  | 2.72                     | 0.57              |
| 35:BI:133:HIS:O   | 35:BI:134:PRO:C   | 2.43                     | 0.57              |
| 38:BP:107:LYS:HG3 | 38:BP:107:LYS:O   | 2.04                     | 0.57              |
| 39:BQ:2:LEU:HG    | 39:BQ:70:PRO:CG   | 2.34                     | 0.57              |
| 39:BQ:46:GLN:O    | 39:BQ:47:ILE:C    | 2.43                     | 0.57              |
| 41:BS:39:ILE:HG22 | 41:BS:39:ILE:O    | 2.05                     | 0.57              |
| 41:BS:42:ASP:O    | 41:BS:43:GLU:HB2  | 2.04                     | 0.57              |
| 41:BS:66:ALA:O    | 41:BS:69:VAL:CG1  | 2.53                     | 0.57              |
| 45:BW:85:VAL:HG12 | 45:BW:86:LEU:H    | 1.69                     | 0.57              |
| 47:BY:13:VAL:HG22 | 47:BY:28:LYS:HE2  | 1.85                     | 0.57              |
| 1:CA:115:G:O2'    | 1:CA:116:A:OP2    | 2.22                     | 0.57              |
| 1:CA:197:A:O2'    | 1:CA:198:G:H8     | 1.87                     | 0.57              |
| 1:CA:19:C:O2      | 1:CA:917:G:C2     | 2.57                     | 0.57              |
| 1:CA:49:U:O2      | 1:CA:362:G:H1'    | 2.05                     | 0.57              |
| 1:CA:527:G:H2'    | 1:CA:528:C:H5'    | 1.85                     | 0.57              |
| 1:CA:723:U:O2'    | 1:CA:724:G:H5'    | 2.05                     | 0.57              |
| 3:CC:127:ARG:NH1  | 3:CC:127:ARG:HG2  | 2.20                     | 0.57              |
| 3:CC:61:ALA:O     | 3:CC:62:ASP:HB2   | 2.05                     | 0.57              |
| 6:CF:8:ILE:HG22   | 6:CF:10:LEU:CD1   | 2.30                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:CL:43:LYS:CG    | 12:CL:44:LYS:N    | 2.61                     | 0.57              |
| 23:CW:70:C:O2'     | 23:CW:71:A:C8     | 2.58                     | 0.57              |
| 53:D4:62:CYS:C     | 53:D4:64:LYS:H    | 2.06                     | 0.57              |
| 57:D8:6:THR:HG22   | 57:D8:63:PRO:CG   | 2.33                     | 0.57              |
| 27:DA:2159:G:C2'   | 27:DA:2160:G:H5'' | 2.34                     | 0.57              |
| 27:DA:265:A:O2'    | 27:DA:266:G:O4'   | 2.23                     | 0.57              |
| 27:DA:292:C:C2     | 27:DA:349:G:N2    | 2.72                     | 0.57              |
| 27:DA:856:C:H4'    | 27:DA:857:C:OP1   | 2.03                     | 0.57              |
| 27:DA:861:A:H2'    | 27:DA:862:G:O4'   | 2.03                     | 0.57              |
| 27:DA:873:G:C2     | 27:DA:905:U:H1'   | 2.39                     | 0.57              |
| 28:DB:44:G:C2      | 28:DB:48:A:C2     | 2.92                     | 0.57              |
| 27:DA:2126:A:C5'   | 29:DC:36:LYS:HG2  | 2.34                     | 0.57              |
| 30:DD:26:LYS:NZ    | 30:DD:82:ILE:HB   | 2.20                     | 0.57              |
| 27:DA:1993:U:H4'   | 31:DE:128:SER:HB3 | 1.85                     | 0.57              |
| 32:DF:125:LEU:HD11 | 32:DF:199:TRP:CD1 | 2.39                     | 0.57              |
| 40:DR:14:SER:HA    | 40:DR:17:ARG:HH12 | 1.69                     | 0.57              |
| 40:DR:26:LYS:NZ    | 40:DR:71:GLN:HB3  | 2.19                     | 0.57              |
| 47:DY:54:LYS:O     | 47:DY:55:TYR:CG   | 2.57                     | 0.57              |
| 1:AA:1113:C:H2'    | 1:AA:1114:C:C6    | 2.40                     | 0.57              |
| 1:AA:1243:C:H2'    | 1:AA:1244:C:H6    | 1.69                     | 0.57              |
| 1:AA:1471:G:H2'    | 1:AA:1472:U:C6    | 2.40                     | 0.57              |
| 1:AA:188:C:O4'     | 20:AT:89:ARG:NH2  | 2.38                     | 0.57              |
| 1:AA:49:U:O2'      | 1:AA:50:A:H2'     | 2.03                     | 0.57              |
| 1:AA:64:G:C4'      | 1:AA:65:U:O5'     | 2.49                     | 0.57              |
| 2:AB:17:PHE:HD2    | 2:AB:17:PHE:N     | 2.02                     | 0.57              |
| 3:AC:64:VAL:HG22   | 3:AC:98:ASN:O     | 2.04                     | 0.57              |
| 5:AE:76:ILE:O      | 5:AE:93:PRO:HB3   | 2.05                     | 0.57              |
| 8:AH:37:ARG:O      | 8:AH:37:ARG:HG2   | 2.04                     | 0.57              |
| 11:AK:28:THR:HG21  | 11:AK:61:ALA:CB   | 2.33                     | 0.57              |
| 13:AM:52:GLU:HG2   | 13:AM:55:ARG:NH2  | 2.20                     | 0.57              |
| 13:AM:82:MET:HG2   | 13:AM:82:MET:O    | 2.04                     | 0.57              |
| 17:AQ:43:LEU:HD12  | 17:AQ:68:ARG:CG   | 2.30                     | 0.57              |
| 17:AQ:63:ARG:NH1   | 17:AQ:63:ARG:HB3  | 2.18                     | 0.57              |
| 25:AY:54:U:H2'     | 25:AY:56:G:OP2    | 2.04                     | 0.57              |
| 52:B3:30:ARG:H     | 52:B3:33:GLN:NE2  | 2.03                     | 0.57              |
| 27:BA:1261:C:C2'   | 27:BA:1262:A:O5'  | 2.53                     | 0.57              |
| 27:BA:1859:A:N6    | 27:BA:1883:G:O2'  | 2.38                     | 0.57              |
| 27:BA:2051:A:H4'   | 27:BA:2052:G:OP1  | 2.04                     | 0.57              |
| 27:BA:2407:G:H2'   | 27:BA:2408:U:C6   | 2.39                     | 0.57              |
| 29:BC:76:ALA:C     | 29:BC:78:ALA:H    | 2.08                     | 0.57              |
| 27:BA:2810:A:C2'   | 31:BE:61:ARG:NH2  | 2.68                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:BF:132:VAL:CG1 | 32:BF:133:ASN:H   | 2.05                     | 0.57              |
| 34:BH:138:LYS:O   | 34:BH:141:VAL:HB  | 2.04                     | 0.57              |
| 37:BO:103:ALA:C   | 37:BO:105:GLU:N   | 2.58                     | 0.57              |
| 39:BQ:39:PRO:O    | 39:BQ:40:ALA:HB2  | 2.04                     | 0.57              |
| 42:BT:40:THR:O    | 42:BT:41:ARG:HB2  | 2.04                     | 0.57              |
| 42:BT:74:ARG:HD2  | 42:BT:76:PHE:CZ   | 2.40                     | 0.57              |
| 48:BZ:39:ASP:OD1  | 48:BZ:41:VAL:HG12 | 2.04                     | 0.57              |
| 1:CA:1060:C:H2'   | 1:CA:1061:G:H8    | 1.69                     | 0.57              |
| 1:CA:968:A:N6     | 1:CA:1063:C:H5'   | 2.19                     | 0.57              |
| 1:CA:53:A:N1      | 1:CA:54:C:C2      | 2.73                     | 0.57              |
| 1:CA:986:A:H2'    | 1:CA:987:G:O4'    | 2.04                     | 0.57              |
| 2:CB:141:GLU:O    | 2:CB:145:LEU:HB2  | 2.05                     | 0.57              |
| 10:CJ:22:LYS:C    | 10:CJ:22:LYS:HD2  | 2.25                     | 0.57              |
| 13:CM:80:ARG:O    | 13:CM:82:MET:N    | 2.38                     | 0.57              |
| 17:CQ:66:SER:OG   | 17:CQ:69:LYS:HB3  | 2.05                     | 0.57              |
| 20:CT:91:LEU:C    | 20:CT:93:GLU:H    | 2.07                     | 0.57              |
| 27:DA:1248:G:H3'  | 27:DA:1249:U:H5'  | 1.86                     | 0.57              |
| 27:DA:220:G:H2'   | 27:DA:221:A:N7    | 2.19                     | 0.57              |
| 27:DA:2896:C:H2'  | 27:DA:2896:C:O2   | 2.04                     | 0.57              |
| 27:DA:720:C:H2'   | 27:DA:721:C:C6    | 2.40                     | 0.57              |
| 27:DA:7:G:H5''    | 36:DN:121:LYS:NZ  | 2.20                     | 0.57              |
| 29:DC:18:LYS:O    | 29:DC:19:VAL:C    | 2.43                     | 0.57              |
| 30:DD:243:GLY:O   | 30:DD:244:ARG:HB3 | 2.04                     | 0.57              |
| 41:DS:61:ASN:O    | 41:DS:62:LYS:HG2  | 2.05                     | 0.57              |
| 43:DU:97:ASP:HA   | 43:DU:100:VAL:CG2 | 2.35                     | 0.57              |
| 1:AA:1378:C:C5'   | 7:AG:94:ARG:HH12  | 2.17                     | 0.57              |
| 1:AA:1525:G:OP1   | 11:AK:120:ARG:NH2 | 2.38                     | 0.57              |
| 2:AB:171:ALA:HA   | 2:AB:174:VAL:CG2  | 2.34                     | 0.57              |
| 2:AB:80:ILE:CD1   | 2:AB:211:ILE:HG22 | 2.35                     | 0.57              |
| 5:AE:43:LEU:HD12  | 5:AE:44:GLY:N     | 2.19                     | 0.57              |
| 8:AH:12:ARG:HD2   | 8:AH:26:VAL:HB    | 1.87                     | 0.57              |
| 8:AH:44:PHE:HE2   | 8:AH:109:ILE:CG2  | 2.17                     | 0.57              |
| 11:AK:18:ARG:NH2  | 11:AK:35:PRO:O    | 2.33                     | 0.57              |
| 17:AQ:62:SER:OG   | 17:AQ:72:ARG:HG3  | 2.05                     | 0.57              |
| 25:AY:18:G:H5'    | 25:AY:19:U:H5     | 1.70                     | 0.57              |
| 27:BA:181:A:C2    | 27:BA:435:C:H5    | 2.23                     | 0.57              |
| 27:BA:1999:C:N3   | 27:BA:2000:G:C8   | 2.73                     | 0.57              |
| 27:BA:2697:G:H2'  | 27:BA:2698:U:O4'  | 2.04                     | 0.57              |
| 27:BA:62:C:H2'    | 27:BA:63:U:H5'    | 1.85                     | 0.57              |
| 27:BA:706:A:H2'   | 27:BA:707:G:O4'   | 2.04                     | 0.57              |
| 27:BA:792:G:H4'   | 27:BA:793:A:O5'   | 2.05                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:6:A:C2       | 27:BA:7:G:C4       | 2.92                     | 0.57              |
| 28:BB:7:G:H21      | 41:BS:38:GLN:NE2   | 2.01                     | 0.57              |
| 30:BD:213:ARG:O    | 30:BD:216:GLY:N    | 2.36                     | 0.57              |
| 31:BE:69:LYS:C     | 31:BE:71:GLY:H     | 2.08                     | 0.57              |
| 31:BE:77:ILE:C     | 31:BE:78:LEU:HD23  | 2.25                     | 0.57              |
| 32:BF:21:ALA:N     | 32:BF:23:ASP:OD1   | 2.38                     | 0.57              |
| 32:BF:78:ILE:H     | 32:BF:78:ILE:HD13  | 1.70                     | 0.57              |
| 34:BH:158:HIS:CD2  | 34:BH:170:ARG:O    | 2.57                     | 0.57              |
| 38:BP:99:LEU:HG    | 38:BP:102:ARG:HH11 | 1.69                     | 0.57              |
| 39:BQ:134:ARG:HH21 | 48:BZ:121:ARG:NH2  | 2.03                     | 0.57              |
| 40:BR:34:ILE:HG22  | 40:BR:35:THR:N     | 2.20                     | 0.57              |
| 40:BR:76:VAL:HG12  | 40:BR:77:ARG:N     | 2.20                     | 0.57              |
| 40:BR:55:ALA:HA    | 40:BR:80:PHE:CE1   | 2.40                     | 0.57              |
| 27:BA:483:A:O2'    | 47:BY:60:PHE:HZ    | 1.87                     | 0.57              |
| 1:CA:269:C:H2'     | 1:CA:270:A:H8      | 1.68                     | 0.57              |
| 1:CA:406:G:H5''    | 4:CD:5:ILE:CG2     | 2.35                     | 0.57              |
| 1:CA:419:C:H2'     | 1:CA:420:U:H5'     | 1.85                     | 0.57              |
| 1:CA:424:G:H8      | 1:CA:424:G:O5'     | 1.88                     | 0.57              |
| 1:CA:428:G:O4'     | 1:CA:430:A:C8      | 2.58                     | 0.57              |
| 1:CA:859:A:C2'     | 1:CA:860:A:H5'     | 2.35                     | 0.57              |
| 1:CA:860:A:H4'     | 8:CH:75:ARG:NH2    | 2.19                     | 0.57              |
| 1:CA:880:C:H2'     | 1:CA:881:G:C8      | 2.36                     | 0.57              |
| 1:CA:895:G:H2'     | 1:CA:896:C:H6      | 1.70                     | 0.57              |
| 2:CB:80:ILE:HG12   | 2:CB:215:LEU:HD12  | 1.87                     | 0.57              |
| 1:CA:619:U:C2      | 4:CD:135:LEU:HD21  | 2.39                     | 0.57              |
| 4:CD:173:TRP:CD1   | 4:CD:189:PRO:HG3   | 2.37                     | 0.57              |
| 1:CA:738:C:H5'     | 6:CF:72:VAL:HG11   | 1.87                     | 0.57              |
| 8:CH:39:LEU:HD12   | 8:CH:44:PHE:CD2    | 2.39                     | 0.57              |
| 27:DA:1233:C:H2'   | 27:DA:1234:U:C6    | 2.39                     | 0.57              |
| 27:DA:1357:U:O2'   | 27:DA:1358:G:H5'   | 2.04                     | 0.57              |
| 27:DA:1550:C:H2'   | 27:DA:1551:C:H6    | 1.67                     | 0.57              |
| 27:DA:1971:A:C4    | 30:DD:241:PRO:HG3  | 2.40                     | 0.57              |
| 27:DA:2003:G:H2'   | 27:DA:2004:G:O5'   | 2.04                     | 0.57              |
| 27:DA:2087:G:O2'   | 27:DA:2088:G:H5'   | 2.05                     | 0.57              |
| 27:DA:2108:C:H2'   | 27:DA:2109:U:H5'   | 1.86                     | 0.57              |
| 27:DA:2183:C:O2'   | 27:DA:2184:G:H5'   | 2.05                     | 0.57              |
| 27:DA:2303:G:H2'   | 27:DA:2304:G:H8    | 1.69                     | 0.57              |
| 27:DA:230:U:H2'    | 27:DA:231:C:H6     | 1.69                     | 0.57              |
| 27:DA:2553:G:H2'   | 27:DA:2554:U:O4'   | 2.03                     | 0.57              |
| 27:DA:378:C:O2'    | 27:DA:379:G:H5'    | 2.05                     | 0.57              |
| 27:DA:620:G:H4'    | 27:DA:621:A:OP1    | 2.04                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:DC:66:HIS:O     | 29:DC:68:LEU:N    | 2.36                     | 0.57              |
| 30:DD:77:ALA:HB3   | 30:DD:117:VAL:CG2 | 2.32                     | 0.57              |
| 33:DG:68:PRO:HA    | 33:DG:92:VAL:HB   | 1.85                     | 0.57              |
| 27:DA:1665:A:C4'   | 37:DO:67:LYS:HB2  | 2.34                     | 0.57              |
| 37:DO:73:ASP:OD1   | 37:DO:75:SER:HB3  | 2.05                     | 0.57              |
| 38:DP:25:SER:O     | 38:DP:27:HIS:N    | 2.37                     | 0.57              |
| 39:DQ:69:PHE:O     | 39:DQ:95:ALA:HB2  | 2.04                     | 0.57              |
| 40:DR:10:LEU:HB3   | 40:DR:17:ARG:CZ   | 2.35                     | 0.57              |
| 40:DR:48:VAL:O     | 40:DR:52:ILE:HG12 | 2.04                     | 0.57              |
| 1:AA:1001(A):G:C8  | 1:AA:1002:G:C8    | 2.92                     | 0.57              |
| 1:AA:1294:G:O2'    | 1:AA:1295:G:H5'   | 2.04                     | 0.57              |
| 1:AA:131:C:OP1     | 1:AA:263:A:H4'    | 2.05                     | 0.57              |
| 1:AA:423:G:C2'     | 1:AA:424:G:H5'    | 2.35                     | 0.57              |
| 1:AA:546:G:OP2     | 4:AD:72:GLU:HB3   | 2.05                     | 0.57              |
| 1:AA:582:U:H2'     | 1:AA:583:A:H8     | 1.70                     | 0.57              |
| 2:AB:53:ARG:NH2    | 2:AB:199:TYR:HE2  | 2.02                     | 0.57              |
| 3:AC:92:ALA:HB2    | 3:AC:99:VAL:CG1   | 2.34                     | 0.57              |
| 4:AD:178:VAL:O     | 4:AD:180:GLY:N    | 2.37                     | 0.57              |
| 5:AE:41:VAL:HG11   | 5:AE:113:ALA:CA   | 2.34                     | 0.57              |
| 6:AF:3:ARG:NH1     | 6:AF:38:GLU:OE1   | 2.38                     | 0.57              |
| 7:AG:31:MET:HG3    | 7:AG:35:LYS:H     | 1.69                     | 0.57              |
| 9:AI:46:ALA:C      | 9:AI:47:LEU:HD12  | 2.25                     | 0.57              |
| 13:AM:104:ARG:HG2  | 13:AM:105:THR:H   | 1.68                     | 0.57              |
| 15:AO:82:ILE:CD1   | 15:AO:87:ILE:H    | 2.15                     | 0.57              |
| 20:AT:22:ARG:O     | 20:AT:26:ASN:ND2  | 2.38                     | 0.57              |
| 25:AY:7:A:N1       | 25:AY:48:C:C4     | 2.73                     | 0.57              |
| 49:B0:41:ARG:H     | 49:B0:41:ARG:HD2  | 1.69                     | 0.57              |
| 50:B1:73:LEU:O     | 50:B1:75:GLU:N    | 2.37                     | 0.57              |
| 55:B6:19:ARG:N     | 55:B6:19:ARG:HD2  | 2.16                     | 0.57              |
| 57:B8:21:LYS:HD3   | 57:B8:48:PHE:CZ   | 2.39                     | 0.57              |
| 57:B8:35:GLN:CG    | 57:B8:35:GLN:O    | 2.53                     | 0.57              |
| 27:BA:1386:C:H2'   | 27:BA:1387:C:C6   | 2.40                     | 0.57              |
| 27:BA:1658:C:H2'   | 27:BA:1659:U:C6   | 2.39                     | 0.57              |
| 27:BA:1661:G:H2'   | 27:BA:1662:C:H6   | 1.69                     | 0.57              |
| 27:BA:1957:C:O2'   | 27:BA:1985:G:H1'  | 2.04                     | 0.57              |
| 27:BA:2692:C:H42   | 27:BA:2717:G:H1   | 1.52                     | 0.57              |
| 27:BA:271(I):G:H3' | 27:BA:271(J):C:C6 | 2.36                     | 0.57              |
| 27:BA:83:G:HO2'    | 27:BA:84:A:H8     | 1.51                     | 0.57              |
| 29:BC:76:ALA:H     | 29:BC:94:VAL:HG12 | 1.69                     | 0.57              |
| 30:BD:71:ASP:HB2   | 30:BD:103:ARG:NH2 | 2.17                     | 0.57              |
| 30:BD:80:ALA:H     | 30:BD:95:LEU:HA   | 1.69                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:BF:3:GLU:CB    | 32:BF:19:GLU:HB2  | 2.16                     | 0.57              |
| 32:BF:2:LYS:HG2   | 32:BF:25:PRO:CB   | 2.35                     | 0.57              |
| 32:BF:53:THR:HB   | 32:BF:56:GLU:CG   | 2.34                     | 0.57              |
| 41:BS:85:VAL:HG23 | 41:BS:106:ARG:HB3 | 1.85                     | 0.57              |
| 42:BT:61:PHE:CE2  | 42:BT:76:PHE:HB2  | 2.39                     | 0.57              |
| 43:BU:26:GLY:C    | 43:BU:28:ARG:N    | 2.49                     | 0.57              |
| 43:BU:47:TYR:HA   | 43:BU:50:ARG:NH2  | 2.19                     | 0.57              |
| 47:BY:67:LEU:HD12 | 47:BY:68:HIS:N    | 2.20                     | 0.57              |
| 1:CA:115:G:H1'    | 1:CA:116:A:N7     | 2.20                     | 0.57              |
| 1:CA:320:C:C1'    | 1:CA:1434:A:H2    | 2.17                     | 0.57              |
| 1:CA:831:U:O2'    | 1:CA:832:C:H5'    | 2.04                     | 0.57              |
| 1:CA:859:A:O2'    | 1:CA:860:A:H5'    | 2.05                     | 0.57              |
| 2:CB:82:ARG:HG3   | 2:CB:92:TYR:HE2   | 1.70                     | 0.57              |
| 7:CG:92:SER:O     | 7:CG:96:GLN:HB2   | 2.04                     | 0.57              |
| 8:CH:39:LEU:HD22  | 8:CH:39:LEU:N     | 2.18                     | 0.57              |
| 10:CJ:12:ASP:HB3  | 10:CJ:15:THR:OG1  | 2.04                     | 0.57              |
| 10:CJ:50:ILE:HG23 | 10:CJ:60:ARG:NH1  | 2.20                     | 0.57              |
| 23:CW:7:A:H5'     | 23:CW:8:U:OP2     | 2.04                     | 0.57              |
| 49:D0:25:ARG:HA   | 49:D0:29:GLN:NE2  | 2.20                     | 0.57              |
| 51:D2:50:ILE:C    | 51:D2:52:ASP:N    | 2.56                     | 0.57              |
| 52:D3:22:ALA:C    | 52:D3:24:LYS:H    | 2.08                     | 0.57              |
| 27:DA:1404:C:O2   | 27:DA:1404:C:H2'  | 2.04                     | 0.57              |
| 27:DA:2061:G:H5'' | 27:DA:2503:A:C2   | 2.39                     | 0.57              |
| 27:DA:2243:U:H2'  | 27:DA:2243:U:O2   | 2.05                     | 0.57              |
| 27:DA:867:C:C4    | 27:DA:868:U:O4    | 2.58                     | 0.57              |
| 27:DA:88:G:H2'    | 27:DA:88:G:N3     | 2.19                     | 0.57              |
| 27:DA:999:U:O2'   | 27:DA:1000:A:H5'' | 2.04                     | 0.57              |
| 28:DB:15:A:H1'    | 28:DB:110:G:N7    | 2.20                     | 0.57              |
| 28:DB:93:G:H2'    | 28:DB:94:C:H6     | 1.70                     | 0.57              |
| 31:DE:60:ASN:CG   | 31:DE:62:PRO:HD2  | 2.25                     | 0.57              |
| 36:DN:32:THR:HG23 | 36:DN:37:LYS:HG2  | 1.87                     | 0.57              |
| 44:DV:19:LYS:HE2  | 44:DV:20:LEU:H    | 1.69                     | 0.57              |
| 47:DY:26:LYS:NZ   | 47:DY:27:VAL:HG23 | 2.20                     | 0.57              |
| 1:AA:103:C:H2'    | 1:AA:104:G:O4'    | 2.04                     | 0.57              |
| 1:AA:1065:U:C5    | 1:AA:1190:G:H1'   | 2.40                     | 0.57              |
| 1:AA:217:C:O2'    | 1:AA:470:C:N4     | 2.38                     | 0.57              |
| 10:AJ:80:LYS:O    | 10:AJ:84:GLN:NE2  | 2.37                     | 0.57              |
| 17:AQ:32:TYR:O    | 17:AQ:34:LYS:N    | 2.37                     | 0.57              |
| 22:AV:8:A:C6      | 22:AV:9:G:C6      | 2.93                     | 0.57              |
| 24:AX:75:C:H2'    | 24:AX:76:A:O4'    | 2.04                     | 0.57              |
| 25:AY:56:G:N3     | 25:AY:56:G:H2'    | 2.19                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:AZ:6:5OH:HS    | 26:AZ:6:5OH:N      | 2.19                     | 0.57              |
| 27:BA:2815:C:C5'  | 54:B5:29:THR:HG21  | 2.35                     | 0.57              |
| 27:BA:1766:U:O2'  | 27:BA:1767:C:H5'   | 2.04                     | 0.57              |
| 27:BA:390:A:H4'   | 27:BA:391:G:O5'    | 2.05                     | 0.57              |
| 27:BA:557:U:H2'   | 27:BA:558:G:C8     | 2.39                     | 0.57              |
| 32:BF:103:LYS:HA  | 32:BF:106:ARG:HG3  | 1.87                     | 0.57              |
| 37:BO:11:ALA:HB3  | 37:BO:85:VAL:HG22  | 1.86                     | 0.57              |
| 42:BT:32:TYR:CD2  | 42:BT:81:PRO:O     | 2.58                     | 0.57              |
| 48:BZ:172:ALA:O   | 48:BZ:173:VAL:HG23 | 2.05                     | 0.57              |
| 1:CA:114:U:H2'    | 1:CA:115:G:C8      | 2.38                     | 0.57              |
| 1:CA:1165:C:O2'   | 1:CA:1166:G:H5'    | 2.05                     | 0.57              |
| 1:CA:527:G:O2'    | 1:CA:528:C:H5'     | 2.04                     | 0.57              |
| 2:CB:131:PRO:O    | 2:CB:135:GLN:N     | 2.34                     | 0.57              |
| 2:CB:142:LEU:O    | 2:CB:146:GLN:HB3   | 2.05                     | 0.57              |
| 3:CC:79:ARG:C     | 3:CC:81:GLY:H      | 2.07                     | 0.57              |
| 12:CL:87:VAL:HG22 | 12:CL:96:HIS:CE1   | 2.38                     | 0.57              |
| 20:CT:28:ALA:C    | 20:CT:30:LYS:H     | 2.08                     | 0.57              |
| 20:CT:31:SER:O    | 20:CT:32:ALA:C     | 2.42                     | 0.57              |
| 27:DA:1257:C:H4'  | 32:DF:83:PHE:CD2   | 2.39                     | 0.57              |
| 27:DA:2056:G:H22  | 54:D5:4:HIS:HA     | 1.69                     | 0.57              |
| 27:DA:954:G:O2'   | 27:DA:2274:A:N1    | 2.33                     | 0.57              |
| 27:DA:2401:U:H2'  | 27:DA:2401:U:O2    | 2.04                     | 0.57              |
| 27:DA:2406:U:H5'' | 27:DA:2408:U:OP2   | 2.05                     | 0.57              |
| 27:DA:2445:G:H2'  | 27:DA:2446:G:H8    | 1.69                     | 0.57              |
| 27:DA:2460:U:H2'  | 27:DA:2461:C:H5'   | 1.87                     | 0.57              |
| 27:DA:2571:C:H5'  | 27:DA:2572:A:H5'   | 1.87                     | 0.57              |
| 27:DA:2728:U:O2'  | 27:DA:2729:G:H5'   | 2.04                     | 0.57              |
| 27:DA:2795:G:N2   | 27:DA:2799:C:H5'   | 2.19                     | 0.57              |
| 27:DA:416:C:C4    | 27:DA:417:C:C4     | 2.92                     | 0.57              |
| 27:DA:784:A:O2'   | 27:DA:785:G:H5''   | 2.05                     | 0.57              |
| 27:DA:90:U:HO2'   | 27:DA:92:A:H5''    | 1.65                     | 0.57              |
| 29:DC:68:LEU:HD11 | 29:DC:179:SER:C    | 2.24                     | 0.57              |
| 33:DG:138:GLN:HB3 | 33:DG:153:ARG:O    | 2.05                     | 0.57              |
| 33:DG:29:TRP:HA   | 33:DG:29:TRP:HE3   | 1.69                     | 0.57              |
| 35:DI:4:ILE:HD11  | 35:DI:44:LEU:HD13  | 1.86                     | 0.57              |
| 36:DN:28:THR:O    | 36:DN:31:ALA:HB3   | 2.05                     | 0.57              |
| 40:DR:14:SER:HA   | 40:DR:17:ARG:NH1   | 2.20                     | 0.57              |
| 31:DE:111:ARG:C   | 40:DR:2:ARG:HG3    | 2.24                     | 0.57              |
| 41:DS:58:LEU:HB3  | 41:DS:65:VAL:HG13  | 1.86                     | 0.57              |
| 41:DS:89:ARG:CB   | 41:DS:92:TYR:HB3   | 2.32                     | 0.57              |
| 44:DV:61:VAL:O    | 44:DV:62:LEU:HD13  | 2.04                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:DX:26:TYR:CZ    | 46:DX:89:ILE:HB   | 2.39                     | 0.57              |
| 47:DY:75:ILE:HG13  | 47:DY:79:CYS:CA   | 2.20                     | 0.57              |
| 48:DZ:38:VAL:HG23  | 48:DZ:39:ASP:N    | 2.20                     | 0.57              |
| 1:AA:70:G:N2       | 1:AA:100:C:C2     | 2.73                     | 0.57              |
| 1:AA:129(A):G:N2   | 1:AA:189(E):U:O2' | 2.38                     | 0.57              |
| 1:AA:756:C:H2'     | 1:AA:757:U:O4'    | 2.04                     | 0.57              |
| 1:AA:826:C:H2'     | 1:AA:827:U:C6     | 2.39                     | 0.57              |
| 6:AF:72:VAL:HG13   | 6:AF:73:ASN:H     | 1.69                     | 0.57              |
| 7:AG:60:LYS:HZ1    | 7:AG:63:LYS:HB3   | 1.70                     | 0.57              |
| 8:AH:84:ARG:HH11   | 8:AH:84:ARG:CB    | 2.16                     | 0.57              |
| 10:AJ:40:LEU:N     | 10:AJ:40:LEU:HD23 | 2.19                     | 0.57              |
| 10:AJ:82:ILE:O     | 10:AJ:82:ILE:HG22 | 2.03                     | 0.57              |
| 12:AL:80:VAL:HG11  | 12:AL:104:ALA:CB  | 2.34                     | 0.57              |
| 16:AP:4:ILE:HA     | 16:AP:20:VAL:O    | 2.05                     | 0.57              |
| 18:AR:40:LEU:O     | 18:AR:42:ARG:N    | 2.38                     | 0.57              |
| 50:B1:51:VAL:O     | 50:B1:51:VAL:HG13 | 2.04                     | 0.57              |
| 27:BA:1273:U:O2'   | 27:BA:1274:A:H5'' | 2.05                     | 0.57              |
| 27:BA:173:G:H2'    | 27:BA:173:G:N3    | 2.20                     | 0.57              |
| 27:BA:2047:U:H2'   | 27:BA:2048:G:C5'  | 2.34                     | 0.57              |
| 27:BA:2732:G:C2'   | 27:BA:2733:A:H5'  | 2.34                     | 0.57              |
| 28:BB:31:C:N4      | 41:BS:32:LEU:HD13 | 2.20                     | 0.57              |
| 30:BD:226:MET:HB3  | 30:BD:230:ASP:CB  | 2.33                     | 0.57              |
| 33:BG:161:THR:HG21 | 33:BG:172:LEU:CD2 | 2.35                     | 0.57              |
| 34:BH:103:LEU:HD21 | 34:BH:105:LEU:CD2 | 2.35                     | 0.57              |
| 36:BN:46:VAL:O     | 36:BN:47:ALA:HB2  | 2.04                     | 0.57              |
| 37:BO:59:LYS:HD3   | 37:BO:89:ASN:OD1  | 2.04                     | 0.57              |
| 42:BT:51:ARG:HG3   | 42:BT:98:LYS:HG3  | 1.85                     | 0.57              |
| 44:BV:62:LEU:HD23  | 44:BV:93:GLU:HB3  | 1.87                     | 0.57              |
| 1:CA:1106:G:H2'    | 1:CA:1107:C:C6    | 2.40                     | 0.57              |
| 1:CA:1336:C:O4'    | 1:CA:1337:G:C2    | 2.58                     | 0.57              |
| 1:CA:1410:G:H2'    | 1:CA:1411:C:H6    | 1.70                     | 0.57              |
| 1:CA:178:C:H2'     | 1:CA:179:A:H8     | 1.68                     | 0.57              |
| 1:CA:349:A:O2'     | 1:CA:350:G:H5'    | 2.03                     | 0.57              |
| 1:CA:770:C:H2'     | 1:CA:771:G:H8     | 1.68                     | 0.57              |
| 1:CA:874:G:HO2'    | 1:CA:875:C:H6     | 1.51                     | 0.57              |
| 1:CA:985:C:O2'     | 1:CA:986:A:H8     | 1.87                     | 0.57              |
| 7:CG:143:ARG:O     | 7:CG:145:ALA:O    | 2.23                     | 0.57              |
| 1:CA:693:G:HO2'    | 7:CG:82:GLY:HA3   | 1.67                     | 0.57              |
| 8:CH:80:ILE:CG2    | 8:CH:82:HIS:O     | 2.53                     | 0.57              |
| 1:CA:1305:G:OP1    | 21:CU:2:GLY:HA3   | 2.05                     | 0.57              |
| 24:CX:19:G:H1      | 33:DG:83:ARG:NH2  | 2.02                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:CZ:6:5OH:HS    | 26:CZ:6:5OH:N     | 2.19                     | 0.57              |
| 55:D6:22:ALA:O    | 55:D6:23:THR:OG1  | 2.21                     | 0.57              |
| 57:D8:54:GLU:HA   | 57:D8:57:ARG:HE   | 1.70                     | 0.57              |
| 27:DA:2136:C:H41  | 27:DA:2156:G:H21  | 1.53                     | 0.57              |
| 27:DA:815:C:H2'   | 27:DA:816:C:H6    | 1.70                     | 0.57              |
| 38:DP:57:THR:OG1  | 38:DP:59:LEU:HB2  | 2.05                     | 0.57              |
| 40:DR:2:ARG:HH21  | 40:DR:5:LYS:NZ    | 2.03                     | 0.57              |
| 40:DR:51:LEU:HB3  | 40:DR:66:VAL:HG13 | 1.87                     | 0.57              |
| 41:DS:71:ARG:O    | 41:DS:74:ALA:HB3  | 2.03                     | 0.57              |
| 42:DT:31:SER:OG   | 42:DT:32:TYR:N    | 2.36                     | 0.57              |
| 1:AA:1082:G:C2'   | 1:AA:1083:U:H5'   | 2.35                     | 0.56              |
| 1:AA:1172:C:H2'   | 1:AA:1173:G:C8    | 2.40                     | 0.56              |
| 1:AA:1265:G:H3'   | 1:AA:1265:G:C8    | 2.40                     | 0.56              |
| 6:AF:100:ASN:HB2  | 18:AR:28:GLU:HA   | 1.84                     | 0.56              |
| 1:AA:1380:U:C5    | 7:AG:3:ARG:HG3    | 2.40                     | 0.56              |
| 8:AH:6:ILE:N      | 8:AH:6:ILE:HD12   | 2.15                     | 0.56              |
| 14:AN:51:GLY:C    | 14:AN:53:LEU:H    | 2.09                     | 0.56              |
| 15:AO:54:ARG:NH1  | 15:AO:58:MET:HE1  | 2.20                     | 0.56              |
| 54:B5:32:PRO:O    | 54:B5:33:CYS:CB   | 2.52                     | 0.56              |
| 55:B6:36:LEU:CB   | 55:B6:50:ARG:NH1  | 2.68                     | 0.56              |
| 57:B8:50:LEU:O    | 57:B8:51:ALA:HB3  | 2.05                     | 0.56              |
| 27:BA:971:C:H2'   | 27:BA:972:G:H5'   | 1.86                     | 0.56              |
| 28:BB:47:C:C2'    | 28:BB:48:A:H5'    | 2.35                     | 0.56              |
| 30:BD:112:GLN:N   | 30:BD:115:GLN:NE2 | 2.53                     | 0.56              |
| 31:BE:37:ARG:HD2  | 31:BE:42:ASP:CG   | 2.25                     | 0.56              |
| 33:BG:170:ARG:NH2 | 33:BG:182:LYS:NZ  | 2.52                     | 0.56              |
| 42:BT:45:PHE:CZ   | 42:BT:65:LYS:HB3  | 2.40                     | 0.56              |
| 45:BW:19:LEU:HB3  | 54:B5:25:LEU:HD11 | 1.86                     | 0.56              |
| 27:BA:1339:G:H5'' | 46:BX:16:LYS:HD3  | 1.87                     | 0.56              |
| 1:CA:976:G:N7     | 1:CA:1359:C:H1'   | 2.20                     | 0.56              |
| 1:CA:355:C:C4     | 1:CA:356:A:N7     | 2.73                     | 0.56              |
| 2:CB:164:VAL:H    | 2:CB:186:ALA:HB2  | 1.70                     | 0.56              |
| 2:CB:187:LEU:HD23 | 2:CB:201:ILE:O    | 2.06                     | 0.56              |
| 1:CA:409:G:OP1    | 4:CD:24:GLU:HG3   | 2.05                     | 0.56              |
| 8:CH:9:MET:O      | 8:CH:13:ILE:HD13  | 2.04                     | 0.56              |
| 10:CJ:48:THR:HA   | 10:CJ:62:HIS:HB3  | 1.86                     | 0.56              |
| 14:CN:26:ARG:HD2  | 14:CN:43:CYS:SG   | 2.45                     | 0.56              |
| 24:CX:8:U:O2      | 24:CX:8:U:H2'     | 2.04                     | 0.56              |
| 50:D1:50:ARG:HG2  | 50:D1:50:ARG:HH11 | 1.69                     | 0.56              |
| 57:D8:11:LYS:HE2  | 57:D8:64:TYR:CE1  | 2.38                     | 0.56              |
| 57:D8:14:VAL:HG22 | 57:D8:15:LYS:N    | 2.20                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1167:U:H1'   | 27:DA:1183:G:H22   | 1.70                     | 0.56              |
| 27:DA:1385:G:HO2'  | 27:DA:1396:U:H6    | 1.50                     | 0.56              |
| 27:DA:1496:A:H8    | 27:DA:1577:C:HO2'  | 1.53                     | 0.56              |
| 27:DA:2139:C:H2'   | 27:DA:2140:C:C6    | 2.40                     | 0.56              |
| 27:DA:2159:G:H2'   | 27:DA:2160:G:H5''  | 1.87                     | 0.56              |
| 27:DA:2258:C:C6    | 27:DA:2426:A:H5'   | 2.39                     | 0.56              |
| 27:DA:2499:C:N4    | 27:DA:2500:U:N3    | 2.53                     | 0.56              |
| 27:DA:30:G:C6      | 27:DA:31:C:N3      | 2.73                     | 0.56              |
| 27:DA:528:A:H2     | 27:DA:2043:C:H4'   | 1.66                     | 0.56              |
| 27:DA:860:U:H2'    | 27:DA:861:A:C8     | 2.39                     | 0.56              |
| 28:DB:15:A:H3'     | 28:DB:16:G:C5'     | 2.35                     | 0.56              |
| 29:DC:52:ARG:NH2   | 29:DC:53:ARG:HH21  | 2.03                     | 0.56              |
| 27:DA:777:A:O2'    | 30:DD:48:ARG:NH2   | 2.38                     | 0.56              |
| 31:DE:134:ILE:CD1  | 31:DE:134:ILE:N    | 2.68                     | 0.56              |
| 32:DF:132:VAL:HG22 | 32:DF:133:ASN:N    | 2.17                     | 0.56              |
| 32:DF:7:TYR:CB     | 32:DF:16:GLY:H     | 2.05                     | 0.56              |
| 32:DF:199:TRP:O    | 32:DF:202:PHE:HB3  | 2.05                     | 0.56              |
| 32:DF:2:LYS:HG2    | 32:DF:25:PRO:CB    | 2.34                     | 0.56              |
| 36:DN:22:THR:HG23  | 36:DN:61:ARG:O     | 2.05                     | 0.56              |
| 44:DV:68:LYS:HD3   | 44:DV:69:LYS:H     | 1.70                     | 0.56              |
| 48:DZ:114:GLY:HA2  | 48:DZ:173:VAL:HG12 | 1.87                     | 0.56              |
| 1:AA:579:G:C5'     | 1:AA:728:A:H1'     | 2.35                     | 0.56              |
| 1:AA:750:G:H1'     | 15:AO:22:THR:OG1   | 2.04                     | 0.56              |
| 1:AA:784:C:H2'     | 1:AA:785:G:O4'     | 2.05                     | 0.56              |
| 1:AA:876:G:H2'     | 1:AA:877:C:C6      | 2.41                     | 0.56              |
| 1:AA:70:G:N2       | 1:AA:99:U:O2       | 2.35                     | 0.56              |
| 3:AC:58:GLU:H      | 3:AC:65:ALA:CB     | 2.17                     | 0.56              |
| 9:AI:95:LYS:HG3    | 9:AI:96:LEU:H      | 1.71                     | 0.56              |
| 12:AL:80:VAL:HA    | 12:AL:102:TYR:CD1  | 2.38                     | 0.56              |
| 23:AW:6:U:H3'      | 23:AW:7:A:C5'      | 2.31                     | 0.56              |
| 27:BA:2759:G:N2    | 27:BA:2760:C:C2    | 2.73                     | 0.56              |
| 27:BA:588:U:H2'    | 27:BA:589:C:C6     | 2.40                     | 0.56              |
| 27:BA:600:G:O3'    | 32:BF:108:LYS:NZ   | 2.37                     | 0.56              |
| 27:BA:942:G:C2'    | 27:BA:943:U:H5'    | 2.35                     | 0.56              |
| 31:BE:117:MET:O    | 31:BE:117:MET:HG2  | 2.05                     | 0.56              |
| 31:BE:2:LYS:HG2    | 31:BE:95:ILE:HG23  | 1.87                     | 0.56              |
| 34:BH:28:GLY:HA3   | 34:BH:79:VAL:CB    | 2.34                     | 0.56              |
| 32:BF:34:TRP:CZ2   | 38:BP:12:ALA:HB2   | 2.40                     | 0.56              |
| 39:BQ:52:VAL:HA    | 39:BQ:55:VAL:CG1   | 2.34                     | 0.56              |
| 42:BT:127:ALA:O    | 42:BT:129:ARG:N    | 2.38                     | 0.56              |
| 44:BV:17:GLY:O     | 44:BV:18:LEU:HB3   | 2.04                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:BY:81:LYS:NZ   | 47:BY:97:ARG:CG   | 2.68                     | 0.56              |
| 48:BZ:144:GLU:CD  | 48:BZ:145:ILE:H   | 2.08                     | 0.56              |
| 1:CA:984:C:N3     | 1:CA:1222:G:C2    | 2.73                     | 0.56              |
| 1:CA:1463:C:O2'   | 1:CA:1464:G:H5'   | 2.05                     | 0.56              |
| 1:CA:1466:C:O2'   | 1:CA:1467:G:H5'   | 2.04                     | 0.56              |
| 1:CA:310:G:H2'    | 1:CA:311:C:C6     | 2.38                     | 0.56              |
| 13:CM:63:THR:HG22 | 13:CM:63:THR:O    | 2.05                     | 0.56              |
| 25:CY:30:A:H2'    | 25:CY:31:U:H5'    | 1.86                     | 0.56              |
| 27:DA:1027:A:N6   | 27:DA:1126:A:H1'  | 2.20                     | 0.56              |
| 27:DA:1823:G:C4   | 27:DA:1824:G:C8   | 2.93                     | 0.56              |
| 27:DA:2063:C:H2'  | 27:DA:2064:C:O4'  | 2.05                     | 0.56              |
| 27:DA:214:G:H1'   | 27:DA:216:A:O2'   | 2.06                     | 0.56              |
| 27:DA:52:A:HO2'   | 27:DA:53:A:H8     | 0.68                     | 0.56              |
| 33:DG:126:ASP:HA  | 33:DG:166:ASP:OD1 | 2.04                     | 0.56              |
| 27:DA:2094:G:OP1  | 35:DI:22:LYS:HD2  | 2.05                     | 0.56              |
| 36:DN:68:GLU:HG2  | 36:DN:88:GLU:OE2  | 2.05                     | 0.56              |
| 37:DO:2:ILE:O     | 37:DO:33:ALA:N    | 2.31                     | 0.56              |
| 48:DZ:135:PHE:HE1 | 48:DZ:137:GLU:HB3 | 1.69                     | 0.56              |
| 1:AA:1095:U:H2'   | 1:AA:1096:C:C6    | 2.40                     | 0.56              |
| 1:AA:11:G:H2'     | 1:AA:12:U:O4'     | 2.05                     | 0.56              |
| 1:AA:1221:G:H4'   | 19:AS:77:THR:HG21 | 1.87                     | 0.56              |
| 1:AA:397:A:H5'    | 1:AA:398:C:OP1    | 2.05                     | 0.56              |
| 1:AA:956:U:H2'    | 1:AA:957:U:O4'    | 2.05                     | 0.56              |
| 1:AA:971:G:H22    | 1:AA:1363(A):A:P  | 2.28                     | 0.56              |
| 4:AD:88:VAL:O     | 4:AD:92:VAL:HG23  | 2.04                     | 0.56              |
| 7:AG:45:ASP:O     | 7:AG:49:ILE:HG12  | 2.06                     | 0.56              |
| 9:AI:33:PHE:O     | 9:AI:36:TYR:HB3   | 2.04                     | 0.56              |
| 12:AL:86:ARG:HH11 | 12:AL:86:ARG:HB2  | 1.70                     | 0.56              |
| 25:AY:53:U:H3     | 25:AY:60:C:H42    | 1.51                     | 0.56              |
| 50:B1:7:ILE:CD1   | 50:B1:7:ILE:N     | 2.67                     | 0.56              |
| 27:BA:1754:C:H2'  | 27:BA:1755:A:C8   | 2.39                     | 0.56              |
| 27:BA:1765:C:H42  | 27:BA:1987:G:H1   | 1.54                     | 0.56              |
| 27:BA:1914:C:H2'  | 27:BA:1915:U:O4'  | 2.05                     | 0.56              |
| 27:BA:2402:C:C2'  | 27:BA:2403:C:H5'  | 2.34                     | 0.56              |
| 27:BA:2685:G:H5'  | 37:BO:68:GLU:CD   | 2.26                     | 0.56              |
| 27:BA:2694:G:H5'  | 27:BA:2694:G:C8   | 2.29                     | 0.56              |
| 27:BA:748:G:C2'   | 27:BA:750:A:N7    | 2.68                     | 0.56              |
| 27:BA:855:G:H2'   | 27:BA:856:C:C6    | 2.40                     | 0.56              |
| 27:BA:894:C:H2'   | 27:BA:895:U:H6    | 1.69                     | 0.56              |
| 30:BD:205:VAL:O   | 30:BD:206:LEU:C   | 2.44                     | 0.56              |
| 27:BA:2303:G:H5'' | 33:BG:126:ASP:HB2 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 34:BH:43:VAL:O    | 34:BH:43:VAL:CG2    | 2.54                     | 0.56              |
| 37:BO:81:ASP:C    | 37:BO:81:ASP:OD2    | 2.42                     | 0.56              |
| 39:BQ:137:TYR:CD2 | 39:BQ:137:TYR:N     | 2.73                     | 0.56              |
| 43:BU:31:SER:O    | 43:BU:33:ARG:N      | 2.37                     | 0.56              |
| 43:BU:88:ILE:C    | 43:BU:90:VAL:H      | 2.06                     | 0.56              |
| 47:BY:76:CYS:CB   | 47:BY:96:ILE:HD11   | 2.36                     | 0.56              |
| 1:CA:332:G:H2'    | 1:CA:333:G:H8       | 1.70                     | 0.56              |
| 1:CA:966:G:O2'    | 1:CA:967:C:O5'      | 2.23                     | 0.56              |
| 5:CE:57:LYS:HG2   | 5:CE:61:TYR:HE2     | 1.68                     | 0.56              |
| 5:CE:57:LYS:HG2   | 5:CE:61:TYR:CE2     | 2.40                     | 0.56              |
| 5:CE:90:VAL:C     | 5:CE:91:LEU:HD12    | 2.26                     | 0.56              |
| 8:CH:29:SER:O     | 8:CH:32:LYS:HB2     | 2.05                     | 0.56              |
| 12:CL:51:LYS:HD2  | 12:CL:51:LYS:N      | 2.19                     | 0.56              |
| 19:CS:10:PHE:CE2  | 19:CS:38:SER:HA     | 2.40                     | 0.56              |
| 19:CS:53:ASN:O    | 19:CS:77:THR:HG22   | 2.04                     | 0.56              |
| 51:D2:65:ASN:O    | 51:D2:68:ARG:HB2    | 2.05                     | 0.56              |
| 57:D8:43:GLN:O    | 57:D8:44:LYS:CD     | 2.54                     | 0.56              |
| 27:DA:1310:G:OP2  | 56:D7:9:ARG:CZ      | 2.54                     | 0.56              |
| 27:DA:1398:C:C5'  | 27:DA:1398:C:C6     | 2.89                     | 0.56              |
| 27:DA:1445:A:H5'  | 27:DA:1445(A):C:OP2 | 2.05                     | 0.56              |
| 27:DA:2091:U:H1'  | 50:D1:47:GLN:OE1    | 2.05                     | 0.56              |
| 27:DA:2235:G:C2   | 27:DA:2236:C:C2     | 2.93                     | 0.56              |
| 27:DA:2297:C:N3   | 27:DA:2320:A:C8     | 2.74                     | 0.56              |
| 27:DA:2329:G:H2'  | 27:DA:2330:G:C8     | 2.40                     | 0.56              |
| 27:DA:2428:G:OP1  | 27:DA:2428:G:H3'    | 2.06                     | 0.56              |
| 27:DA:2494:G:C2'  | 27:DA:2495:G:O5'    | 2.53                     | 0.56              |
| 27:DA:350:U:O2'   | 27:DA:351:G:H5'     | 2.05                     | 0.56              |
| 29:DC:77:ILE:HG23 | 29:DC:77:ILE:O      | 2.03                     | 0.56              |
| 30:DD:79:VAL:HG12 | 30:DD:113:VAL:HA    | 1.86                     | 0.56              |
| 32:DF:24:LEU:HB3  | 32:DF:25:PRO:CD     | 2.35                     | 0.56              |
| 27:DA:6:A:O2'     | 36:DN:130:HIS:HB3   | 2.06                     | 0.56              |
| 37:DO:65:THR:O    | 37:DO:79:PHE:HD1    | 1.88                     | 0.56              |
| 41:DS:19:LYS:C    | 41:DS:20:ARG:HD3    | 2.24                     | 0.56              |
| 1:AA:1003:G:N2    | 1:AA:1039:C:H42     | 2.03                     | 0.56              |
| 1:AA:1074:G:O3'   | 2:AB:103:THR:HG21   | 2.05                     | 0.56              |
| 1:AA:1143:G:H2'   | 1:AA:1144:G:C8      | 2.40                     | 0.56              |
| 1:AA:1200:C:O2'   | 1:AA:1201:A:OP2     | 2.23                     | 0.56              |
| 1:AA:376:G:H2'    | 1:AA:377:G:H8       | 1.70                     | 0.56              |
| 1:AA:498:U:HO2'   | 1:AA:499:A:P        | 2.28                     | 0.56              |
| 1:AA:731:G:OP1    | 1:AA:766:A:H1'      | 2.06                     | 0.56              |
| 1:AA:769:G:O2'    | 1:AA:770:C:H5'      | 2.05                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:AC:134:ILE:C     | 3:AC:136:GLN:H    | 2.07                     | 0.56              |
| 3:AC:153:VAL:HG22  | 3:AC:198:VAL:HG13 | 1.86                     | 0.56              |
| 7:AG:76:ARG:HB2    | 7:AG:89:MET:SD    | 2.45                     | 0.56              |
| 1:AA:728:A:C5      | 15:AO:54:ARG:HD2  | 2.40                     | 0.56              |
| 1:AA:530:G:O2'     | 23:AW:34:U:H4'    | 2.05                     | 0.56              |
| 27:BA:1445:A:N3    | 27:BA:1445:A:H2'  | 2.19                     | 0.56              |
| 27:BA:1936:A:C3'   | 27:BA:1937:A:C5'  | 2.83                     | 0.56              |
| 27:BA:2096:U:H2'   | 27:BA:2097:C:C6   | 2.40                     | 0.56              |
| 27:BA:2577:A:H2'   | 27:BA:2614:A:N6   | 2.20                     | 0.56              |
| 27:BA:353:G:O2'    | 27:BA:354:G:H5'   | 2.05                     | 0.56              |
| 27:BA:470:A:H2'    | 27:BA:471:A:H8    | 1.70                     | 0.56              |
| 27:BA:64:A:C5      | 46:BX:66:LEU:HD12 | 2.40                     | 0.56              |
| 27:BA:811:U:H3     | 27:BA:1250:G:P    | 2.28                     | 0.56              |
| 31:BE:34:VAL:HG23  | 31:BE:34:VAL:O    | 2.05                     | 0.56              |
| 31:BE:81:ILE:O     | 31:BE:81:ILE:CG2  | 2.53                     | 0.56              |
| 33:BG:123:ASN:HB3  | 33:BG:126:ASP:OD2 | 2.05                     | 0.56              |
| 33:BG:86:MET:CB    | 33:BG:87:PRO:HD3  | 2.35                     | 0.56              |
| 35:BI:114:LEU:HD23 | 35:BI:130:TYR:HE1 | 1.68                     | 0.56              |
| 35:BI:12:LEU:HD23  | 35:BI:12:LEU:N    | 2.21                     | 0.56              |
| 27:BA:2415:G:H4'   | 38:BP:67:MET:N    | 2.21                     | 0.56              |
| 44:BV:57:VAL:O     | 44:BV:57:VAL:HG13 | 2.06                     | 0.56              |
| 46:BX:28:PHE:O     | 46:BX:30:VAL:HG12 | 2.06                     | 0.56              |
| 47:BY:32:PRO:C     | 47:BY:34:LYS:N    | 2.59                     | 0.56              |
| 48:BZ:7:TYR:HB2    | 48:BZ:37:TYR:CE2  | 2.41                     | 0.56              |
| 1:CA:1038:C:H2'    | 1:CA:1039:C:C2    | 2.39                     | 0.56              |
| 1:CA:1194:U:H4'    | 5:CE:22:GLY:O     | 2.06                     | 0.56              |
| 1:CA:1260:C:C3'    | 1:CA:1260:C:C6    | 2.89                     | 0.56              |
| 1:CA:769:G:H4'     | 1:CA:1513:A:H4'   | 1.88                     | 0.56              |
| 1:CA:279:A:HO2'    | 1:CA:280:C:P      | 2.28                     | 0.56              |
| 1:CA:522:C:H41     | 12:CL:50:ARG:NH2  | 2.02                     | 0.56              |
| 1:CA:296:U:H4'     | 1:CA:556:C:O2     | 2.05                     | 0.56              |
| 1:CA:66:G:H2'      | 1:CA:66:G:N3      | 2.21                     | 0.56              |
| 1:CA:940:C:O2'     | 1:CA:941:G:H5'    | 2.06                     | 0.56              |
| 4:CD:18:LYS:HG3    | 4:CD:31:CYS:SG    | 2.45                     | 0.56              |
| 4:CD:46:LYS:O      | 4:CD:47:ARG:C     | 2.43                     | 0.56              |
| 8:CH:5:PRO:O       | 8:CH:8:ASP:HB3    | 2.04                     | 0.56              |
| 8:CH:86:ILE:HB     | 8:CH:133:LEU:HD22 | 1.87                     | 0.56              |
| 9:CI:48:GLU:N      | 9:CI:49:PRO:CD    | 2.69                     | 0.56              |
| 10:CJ:81:THR:C     | 10:CJ:83:GLU:H    | 2.09                     | 0.56              |
| 19:CS:29:ARG:HD2   | 19:CS:30:LEU:N    | 2.21                     | 0.56              |
| 51:D2:31:GLU:O     | 51:D2:34:GLU:HB3  | 2.04                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 57:D8:8:LYS:O     | 57:D8:12:LYS:HG3  | 2.05                     | 0.56              |
| 57:D8:31:HIS:O    | 57:D8:32:LEU:O    | 2.23                     | 0.56              |
| 27:DA:2756:U:H5'' | 58:D9:19:ARG:HA   | 1.86                     | 0.56              |
| 27:DA:1025:G:O2'  | 27:DA:1026:U:P    | 2.64                     | 0.56              |
| 27:DA:1400:G:H2'  | 27:DA:1401:G:C8   | 2.38                     | 0.56              |
| 27:DA:142:A:C8    | 27:DA:1595:G:N2   | 2.66                     | 0.56              |
| 27:DA:1028:A:H2   | 27:DA:2486:G:N3   | 2.03                     | 0.56              |
| 27:DA:506:G:H5''  | 27:DA:507:A:OP1   | 2.05                     | 0.56              |
| 27:DA:582:G:C2    | 27:DA:1259:G:C2   | 2.94                     | 0.56              |
| 28:DB:47:C:H2'    | 28:DB:48:A:H5'    | 1.87                     | 0.56              |
| 30:DD:117:VAL:O   | 30:DD:118:VAL:HB  | 2.05                     | 0.56              |
| 38:DP:127:ALA:HB3 | 38:DP:130:PHE:CE2 | 2.40                     | 0.56              |
| 41:DS:89:ARG:O    | 41:DS:92:TYR:HB3  | 2.05                     | 0.56              |
| 42:DT:35:LYS:HZ1  | 42:DT:41:ARG:HH21 | 1.52                     | 0.56              |
| 43:DU:85:LYS:C    | 43:DU:87:GLY:H    | 2.09                     | 0.56              |
| 48:DZ:97:MET:HE2  | 48:DZ:98:TYR:O    | 2.05                     | 0.56              |
| 1:AA:1131:G:H2'   | 1:AA:1132:C:C5    | 2.41                     | 0.56              |
| 1:AA:192:U:O3'    | 20:AT:57:ARG:HD2  | 2.05                     | 0.56              |
| 1:AA:279:A:H5''   | 1:AA:281:G:H5'    | 1.86                     | 0.56              |
| 1:AA:655:A:H2'    | 1:AA:656:C:H6     | 1.71                     | 0.56              |
| 1:AA:979:C:H2'    | 1:AA:980:C:H5''   | 1.88                     | 0.56              |
| 2:AB:188:ALA:HB1  | 2:AB:192:SER:HB2  | 1.87                     | 0.56              |
| 3:AC:42:LEU:O     | 3:AC:45:LYS:HB2   | 2.04                     | 0.56              |
| 3:AC:67:THR:HG23  | 3:AC:102:ASN:HB2  | 1.86                     | 0.56              |
| 4:AD:8:VAL:C      | 4:AD:10:ARG:N     | 2.59                     | 0.56              |
| 6:AF:10:LEU:CD1   | 6:AF:10:LEU:N     | 2.66                     | 0.56              |
| 12:AL:80:VAL:CG1  | 12:AL:104:ALA:HB3 | 2.34                     | 0.56              |
| 13:AM:49:THR:OG1  | 13:AM:52:GLU:HG3  | 2.05                     | 0.56              |
| 16:AP:74:LEU:HB3  | 16:AP:79:VAL:HG21 | 1.87                     | 0.56              |
| 19:AS:37:ARG:HD3  | 19:AS:37:ARG:O    | 2.06                     | 0.56              |
| 25:AY:24:C:O2'    | 25:AY:25:A:H5'    | 2.05                     | 0.56              |
| 27:BA:75:G:H4'    | 51:B2:55:ARG:NH1  | 2.21                     | 0.56              |
| 51:B2:9:GLN:HE22  | 51:B2:56:GLN:CG   | 2.19                     | 0.56              |
| 55:B6:36:LEU:C    | 55:B6:37:ARG:HD2  | 2.25                     | 0.56              |
| 58:B9:24:TYR:CE2  | 58:B9:35:ARG:CD   | 2.89                     | 0.56              |
| 27:BA:104:U:H2'   | 27:BA:105:C:O4'   | 2.05                     | 0.56              |
| 27:BA:2082:A:H2'  | 27:BA:2083:G:O4'  | 2.05                     | 0.56              |
| 27:BA:639:U:H2'   | 27:BA:640:C:C5    | 2.40                     | 0.56              |
| 27:BA:764:A:C5    | 30:BD:209:ALA:CB  | 2.88                     | 0.56              |
| 27:BA:897:C:C2'   | 27:BA:897:C:O2    | 2.52                     | 0.56              |
| 30:BD:227:ASN:O   | 30:BD:230:ASP:HB2 | 2.03                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BN:57:ALA:O     | 36:BN:58:ASP:OD1   | 2.24                     | 0.56              |
| 38:BP:51:PHE:HB3   | 38:BP:52:GLU:HG2   | 1.87                     | 0.56              |
| 43:BU:101:ARG:O    | 43:BU:102:GLU:HG2  | 2.06                     | 0.56              |
| 43:BU:52:ARG:HD2   | 43:BU:55:ARG:HH21  | 1.70                     | 0.56              |
| 44:BV:37:VAL:O     | 44:BV:38:LEU:HB2   | 2.05                     | 0.56              |
| 1:CA:1377:A:H2'    | 7:CG:7:ALA:HB2     | 1.88                     | 0.56              |
| 1:CA:1380:U:C4     | 7:CG:3:ARG:HG3     | 2.41                     | 0.56              |
| 1:CA:192:U:H2'     | 1:CA:193:C:C6      | 2.41                     | 0.56              |
| 5:CE:103:GLY:C     | 5:CE:105:VAL:H     | 2.09                     | 0.56              |
| 9:CI:8:GLY:O       | 9:CI:14:VAL:HG13   | 2.05                     | 0.56              |
| 20:CT:75:ASN:N     | 20:CT:75:ASN:OD1   | 2.37                     | 0.56              |
| 23:CW:38:U:H2'     | 23:CW:39:C:H6      | 1.70                     | 0.56              |
| 54:D5:4:HIS:CB     | 54:D5:5:PRO:CD     | 2.84                     | 0.56              |
| 55:D6:36:LEU:C     | 55:D6:37:ARG:HD2   | 2.26                     | 0.56              |
| 27:DA:686:G:C2     | 56:D7:11:LYS:HE3   | 2.41                     | 0.56              |
| 27:DA:1313:U:H2'   | 27:DA:1610:A:C2    | 2.41                     | 0.56              |
| 27:DA:2276:G:O2'   | 27:DA:2277:G:C8    | 2.58                     | 0.56              |
| 27:DA:870:A:C2     | 27:DA:908:C:N3     | 2.73                     | 0.56              |
| 30:DD:112:GLN:HB2  | 30:DD:115:GLN:HE21 | 1.69                     | 0.56              |
| 31:DE:110:GLY:CA   | 31:DE:162:ALA:H    | 2.17                     | 0.56              |
| 32:DF:183:VAL:HA   | 32:DF:186:ILE:HG13 | 1.88                     | 0.56              |
| 34:DH:105:LEU:HD23 | 34:DH:115:VAL:CG2  | 2.35                     | 0.56              |
| 37:DO:87:ILE:CG2   | 37:DO:91:LEU:HA    | 2.34                     | 0.56              |
| 38:DP:144:GLU:HG2  | 38:DP:144:GLU:O    | 2.06                     | 0.56              |
| 43:DU:26:GLY:O     | 43:DU:30:LYS:HG2   | 2.05                     | 0.56              |
| 47:DY:27:VAL:CA    | 47:DY:28:LYS:NZ    | 2.64                     | 0.56              |
| 1:AA:1510:U:H3     | 1:AA:1525:G:H1     | 1.54                     | 0.56              |
| 1:AA:344:A:H4'     | 1:AA:345:C:OP2     | 2.04                     | 0.56              |
| 1:AA:663:A:H2'     | 1:AA:664:G:O4'     | 2.04                     | 0.56              |
| 1:AA:803:G:H2'     | 1:AA:804:U:C6      | 2.41                     | 0.56              |
| 2:AB:204:ASN:ND2   | 2:AB:205:ASP:N     | 2.53                     | 0.56              |
| 3:AC:7:PRO:O       | 3:AC:11:ARG:HG2    | 2.06                     | 0.56              |
| 3:AC:200:ALA:C     | 3:AC:201:TYR:CD1   | 2.79                     | 0.56              |
| 4:AD:170:VAL:CG1   | 4:AD:174:LEU:HB2   | 2.35                     | 0.56              |
| 5:AE:129:ILE:O     | 5:AE:130:ASN:C     | 2.44                     | 0.56              |
| 6:AF:15:ASP:O      | 6:AF:17:SER:N      | 2.39                     | 0.56              |
| 16:AP:22:THR:OG1   | 16:AP:23:ASP:N     | 2.38                     | 0.56              |
| 16:AP:28:ARG:HG2   | 16:AP:29:ASP:OD2   | 2.06                     | 0.56              |
| 16:AP:58:TYR:O     | 16:AP:62:VAL:HG22  | 2.05                     | 0.56              |
| 1:AA:262:A:C5'     | 20:AT:74:LYS:HG3   | 2.32                     | 0.56              |
| 51:B2:54:LYS:O     | 51:B2:57:ILE:HB    | 2.05                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1485:G:H2'  | 27:BA:1486:A:C8    | 2.41                     | 0.56              |
| 27:BA:1788:C:O2'  | 27:BA:1789:A:H5'   | 2.05                     | 0.56              |
| 27:BA:1925:C:O2'  | 27:BA:1926:U:H5'   | 2.05                     | 0.56              |
| 27:BA:2160:G:H2'  | 27:BA:2161:C:C5    | 2.41                     | 0.56              |
| 27:BA:2184:G:C6   | 27:BA:2185:C:N4    | 2.73                     | 0.56              |
| 27:BA:330:A:O2'   | 27:BA:331:A:C8     | 2.58                     | 0.56              |
| 27:BA:394:A:H2'   | 27:BA:395:U:O4'    | 2.05                     | 0.56              |
| 27:BA:511:U:C5    | 27:BA:512:G:C5     | 2.94                     | 0.56              |
| 27:BA:535:C:O2'   | 27:BA:536:A:H5'    | 2.05                     | 0.56              |
| 27:BA:549:G:C2'   | 27:BA:551:G:H5''   | 2.35                     | 0.56              |
| 30:BD:142:VAL:CG2 | 30:BD:143:HIS:N    | 2.67                     | 0.56              |
| 31:BE:93:VAL:O    | 31:BE:95:ILE:N     | 2.38                     | 0.56              |
| 32:BF:24:LEU:O    | 32:BF:26:ALA:N     | 2.39                     | 0.56              |
| 32:BF:47:GLY:HA3  | 32:BF:95:ARG:O     | 2.05                     | 0.56              |
| 33:BG:86:MET:CB   | 33:BG:87:PRO:CD    | 2.84                     | 0.56              |
| 34:BH:156:ALA:HB3 | 34:BH:159:GLU:HB3  | 1.88                     | 0.56              |
| 35:BI:127:VAL:HA  | 35:BI:139:GLN:HA   | 1.86                     | 0.56              |
| 40:BR:41:ALA:O    | 40:BR:42:LYS:C     | 2.44                     | 0.56              |
| 42:BT:106:SER:HA  | 42:BT:110:ILE:HG13 | 1.88                     | 0.56              |
| 1:CA:1095:U:H5'   | 1:CA:1109:C:O2     | 2.06                     | 0.56              |
| 1:CA:338:A:H2'    | 1:CA:339:C:O4'     | 2.05                     | 0.56              |
| 1:CA:429:U:H1'    | 1:CA:430:A:H5''    | 1.87                     | 0.56              |
| 1:CA:606:G:H3'    | 1:CA:607:A:H5'     | 1.86                     | 0.56              |
| 1:CA:70:G:O2'     | 1:CA:71:C:H5'      | 2.06                     | 0.56              |
| 1:CA:909:A:H2'    | 1:CA:910:C:O4'     | 2.06                     | 0.56              |
| 10:CJ:96:ILE:H    | 10:CJ:96:ILE:HD13  | 1.70                     | 0.56              |
| 25:CY:61:C:H2'    | 25:CY:62:U:C6      | 2.41                     | 0.56              |
| 27:DA:1140:C:H5'' | 36:DN:66:LYS:NZ    | 2.19                     | 0.56              |
| 27:DA:1011:G:C2   | 27:DA:1151:G:C2    | 2.94                     | 0.56              |
| 27:DA:1650:G:N2   | 27:DA:1651:G:H1'   | 2.21                     | 0.56              |
| 27:DA:1762:A:C8   | 27:DA:1762:A:O5'   | 2.47                     | 0.56              |
| 27:DA:2571:C:C3'  | 27:DA:2572:A:H5'   | 2.36                     | 0.56              |
| 27:DA:2645:G:C4'  | 27:DA:2732:G:O2'   | 2.50                     | 0.56              |
| 27:DA:29:U:O2'    | 27:DA:30:G:H5'     | 2.06                     | 0.56              |
| 27:DA:541:C:H2'   | 27:DA:542:C:C6     | 2.40                     | 0.56              |
| 27:DA:547:A:N3    | 27:DA:547:A:H2'    | 2.21                     | 0.56              |
| 27:DA:58:G:N2     | 27:DA:70:G:C5      | 2.73                     | 0.56              |
| 27:DA:904:C:C2'   | 27:DA:905:U:H5'    | 2.30                     | 0.56              |
| 27:DA:995:C:O2    | 36:DN:4:TYR:OH     | 2.23                     | 0.56              |
| 27:DA:1819:A:C5'  | 30:DD:158:ALA:HB2  | 2.35                     | 0.56              |
| 27:DA:1798:U:H5'' | 30:DD:259:THR:HG22 | 1.83                     | 0.56              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 30:DD:271:ILE:O   | 30:DD:272:ALA:HB2   | 2.05                     | 0.56              |
| 31:DE:3:GLY:O     | 31:DE:4:ILE:HB      | 2.05                     | 0.56              |
| 34:DH:130:ARG:HD3 | 34:DH:132:ARG:NH2   | 2.19                     | 0.56              |
| 27:DA:1006:C:H1'  | 36:DN:106:MET:SD    | 2.46                     | 0.56              |
| 38:DP:85:LEU:HD23 | 38:DP:85:LEU:H      | 1.69                     | 0.56              |
| 27:DA:1242:A:C6   | 38:DP:8:PRO:HB3     | 2.40                     | 0.56              |
| 39:DQ:17:LEU:HD22 | 39:DQ:96:VAL:HG13   | 1.88                     | 0.56              |
| 39:DQ:74:TYR:H    | 39:DQ:90:VAL:HG13   | 1.70                     | 0.56              |
| 40:DR:118:GLU:HA  | 40:DR:118:GLU:OE1   | 2.05                     | 0.56              |
| 40:DR:77:ARG:C    | 40:DR:79:LEU:H      | 2.09                     | 0.56              |
| 42:DT:117:ASP:OD2 | 42:DT:120:ARG:HG3   | 2.05                     | 0.56              |
| 43:DU:103:PRO:O   | 43:DU:106:PHE:N     | 2.39                     | 0.56              |
| 43:DU:108:GLU:O   | 43:DU:111:GLU:HB2   | 2.04                     | 0.56              |
| 44:DV:19:LYS:HZ2  | 44:DV:20:LEU:C      | 2.09                     | 0.56              |
| 45:DW:87:PRO:O    | 45:DW:88:ARG:HD2    | 2.05                     | 0.56              |
| 46:DX:44:GLU:HG2  | 46:DX:49:VAL:O      | 2.05                     | 0.56              |
| 46:DX:89:ILE:HG22 | 46:DX:89:ILE:O      | 2.03                     | 0.56              |
| 47:DY:8:LYS:H     | 47:DY:8:LYS:HD2     | 1.69                     | 0.56              |
| 1:AA:1039:C:O2'   | 1:AA:1040:U:H5'     | 2.04                     | 0.56              |
| 1:AA:1164:G:H2'   | 1:AA:1165:C:C6      | 2.40                     | 0.56              |
| 1:AA:1241:G:O2'   | 1:AA:1242:C:C6      | 2.50                     | 0.56              |
| 1:AA:419:C:C2'    | 1:AA:420:U:H5'      | 2.34                     | 0.56              |
| 1:AA:874:G:H2'    | 1:AA:875:C:H6       | 1.69                     | 0.56              |
| 1:AA:913:A:H4'    | 1:AA:914:A:O5'      | 2.06                     | 0.56              |
| 1:AA:426:G:P      | 4:AD:36:ARG:HH21    | 2.28                     | 0.56              |
| 7:AG:127:ALA:O    | 7:AG:129:GLU:N      | 2.39                     | 0.56              |
| 11:AK:88:GLY:C    | 11:AK:90:GLY:H      | 2.08                     | 0.56              |
| 45:BW:19:LEU:HB3  | 54:B5:25:LEU:CD1    | 2.35                     | 0.56              |
| 27:BA:1019:U:H3   | 27:BA:1142(A):A:H62 | 1.52                     | 0.56              |
| 27:BA:1199:U:H2'  | 27:BA:1200:C:C6     | 2.41                     | 0.56              |
| 27:BA:11:G:O2'    | 27:BA:12:U:H5'      | 2.05                     | 0.56              |
| 27:BA:1281:G:C2   | 27:BA:1290:C:N3     | 2.74                     | 0.56              |
| 27:BA:1316:U:H2'  | 27:BA:1317:A:C8     | 2.39                     | 0.56              |
| 27:BA:1612:C:H42  | 27:BA:1619:G:H1     | 1.54                     | 0.56              |
| 27:BA:247:G:O6    | 57:B8:8:LYS:HB3     | 2.06                     | 0.56              |
| 27:BA:2835:A:H4'  | 27:BA:2836:U:OP1    | 2.05                     | 0.56              |
| 27:BA:2868:A:H2'  | 27:BA:2869:G:C8     | 2.41                     | 0.56              |
| 27:BA:828:U:C5    | 27:BA:829:A:N6      | 2.74                     | 0.56              |
| 27:BA:873:G:C2    | 27:BA:905:U:O2      | 2.59                     | 0.56              |
| 29:BC:196:LEU:O   | 29:BC:198:ALA:N     | 2.39                     | 0.56              |
| 32:BF:65:TRP:CZ3  | 32:BF:72:ARG:HB3    | 2.40                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BG:144:ILE:O    | 33:BG:144:ILE:HG23 | 2.04                     | 0.56              |
| 33:BG:15:VAL:HG22  | 33:BG:175:LEU:HB3  | 1.86                     | 0.56              |
| 34:BH:117:PRO:HB3  | 34:BH:123:PHE:CE1  | 2.41                     | 0.56              |
| 41:BS:29:PHE:O     | 41:BS:35:ILE:HA    | 2.05                     | 0.56              |
| 41:BS:85:VAL:C     | 41:BS:106:ARG:HG3  | 2.26                     | 0.56              |
| 44:BV:52:VAL:HG22  | 44:BV:52:VAL:O     | 2.04                     | 0.56              |
| 48:BZ:156:LEU:HD12 | 48:BZ:156:LEU:N    | 2.20                     | 0.56              |
| 1:CA:1009:G:N2     | 1:CA:1021:G:H1'    | 2.20                     | 0.56              |
| 1:CA:1053:G:C5     | 1:CA:1199:U:H2'    | 2.41                     | 0.56              |
| 1:CA:1423:G:H2'    | 1:CA:1424:C:C6     | 2.41                     | 0.56              |
| 1:CA:189(L):G:H2'  | 1:CA:190:U:C5      | 2.37                     | 0.56              |
| 1:CA:328:C:H2'     | 1:CA:328:C:O2      | 2.05                     | 0.56              |
| 1:CA:898:G:H22     | 1:CA:900:A:H3'     | 1.71                     | 0.56              |
| 2:CB:91:PRO:HA     | 2:CB:151:GLY:O     | 2.05                     | 0.56              |
| 5:CE:33:VAL:HG22   | 5:CE:43:LEU:HD13   | 1.87                     | 0.56              |
| 11:CK:101:SER:C    | 11:CK:103:LEU:N    | 2.56                     | 0.56              |
| 12:CL:112:LYS:O    | 12:CL:114:ARG:N    | 2.38                     | 0.56              |
| 12:CL:67:ILE:HD11  | 12:CL:74:LEU:HD12  | 1.86                     | 0.56              |
| 13:CM:56:LEU:C     | 13:CM:56:LEU:HD13  | 2.26                     | 0.56              |
| 15:CO:4:THR:HG23   | 15:CO:7:GLU:OE2    | 2.06                     | 0.56              |
| 54:D5:40:LYS:HD2   | 54:D5:40:LYS:C     | 2.25                     | 0.56              |
| 54:D5:51:TYR:HD1   | 54:D5:52:TYR:CE2   | 2.23                     | 0.56              |
| 55:D6:14:THR:O     | 55:D6:49:HIS:HA    | 2.05                     | 0.56              |
| 57:D8:50:LEU:O     | 57:D8:51:ALA:HB3   | 2.06                     | 0.56              |
| 57:D8:61:LEU:HD13  | 57:D8:62:LEU:H     | 1.70                     | 0.56              |
| 27:DA:1419:A:H2'   | 27:DA:1421:G:N7    | 2.20                     | 0.56              |
| 27:DA:1639:U:H4'   | 27:DA:2699:C:H4'   | 1.87                     | 0.56              |
| 27:DA:2131:G:H5'   | 27:DA:2133:G:O5'   | 2.06                     | 0.56              |
| 27:DA:2303:G:H1    | 27:DA:2313:C:N4    | 2.04                     | 0.56              |
| 27:DA:2665:A:O2'   | 27:DA:2666:C:H5'   | 2.06                     | 0.56              |
| 27:DA:2747:G:N2    | 27:DA:2748:A:N6    | 2.54                     | 0.56              |
| 27:DA:2848:G:N2    | 27:DA:2867:G:H1'   | 2.19                     | 0.56              |
| 27:DA:522:G:O2'    | 27:DA:523:C:H5'    | 2.06                     | 0.56              |
| 27:DA:99:U:O2'     | 27:DA:100:G:P      | 2.63                     | 0.56              |
| 28:DB:62:C:H2'     | 28:DB:63:G:O4'     | 2.05                     | 0.56              |
| 27:DA:1693:U:O2'   | 30:DD:14:ARG:NH2   | 2.39                     | 0.56              |
| 36:DN:62:VAL:HG22  | 36:DN:66:LYS:HD2   | 1.86                     | 0.56              |
| 37:DO:1:MET:HG3    | 37:DO:32:TYR:CG    | 2.40                     | 0.56              |
| 38:DP:95:VAL:HG23  | 38:DP:100:LEU:HD21 | 1.87                     | 0.56              |
| 39:DQ:27:VAL:N     | 39:DQ:137:TYR:HD1  | 2.00                     | 0.56              |
| 42:DT:27:THR:O     | 42:DT:28:VAL:CG2   | 2.53                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:956:U:O2     | 1:AA:1225:A:C2    | 2.59                     | 0.56              |
| 1:AA:1321:C:H3'   | 1:AA:1322:C:C6    | 2.41                     | 0.56              |
| 1:AA:978:A:C8     | 1:AA:978:A:H5''   | 2.41                     | 0.56              |
| 2:AB:63:MET:HB3   | 2:AB:225:ALA:CB   | 2.33                     | 0.56              |
| 7:AG:43:PHE:C     | 7:AG:43:PHE:CD1   | 2.78                     | 0.56              |
| 8:AH:69:ARG:HB2   | 8:AH:69:ARG:CZ    | 2.36                     | 0.56              |
| 9:AI:105:ASP:OD2  | 9:AI:107:ARG:HD3  | 2.06                     | 0.56              |
| 9:AI:125:TYR:CZ   | 9:AI:127:LYS:HB2  | 2.41                     | 0.56              |
| 51:B2:9:GLN:HE22  | 51:B2:56:GLN:CD   | 2.09                     | 0.56              |
| 57:B8:34:TRP:CE2  | 57:B8:35:GLN:HB3  | 2.41                     | 0.56              |
| 27:BA:1462:C:H2'  | 27:BA:1463:C:O4'  | 2.05                     | 0.56              |
| 27:BA:1491:G:P    | 27:BA:1494:A:N6   | 2.79                     | 0.56              |
| 27:BA:1499:C:C2'  | 27:BA:1500:G:H5'  | 2.34                     | 0.56              |
| 27:BA:2082:A:C8   | 27:BA:2083:G:C8   | 2.94                     | 0.56              |
| 27:BA:2804:C:H2'  | 27:BA:2805:G:C8   | 2.41                     | 0.56              |
| 27:BA:834:C:O2'   | 27:BA:835:A:H5'   | 2.06                     | 0.56              |
| 30:BD:146:GLU:OE2 | 30:BD:152:GLY:N   | 2.37                     | 0.56              |
| 27:BA:2682:U:H5'' | 31:BE:11:MET:O    | 2.05                     | 0.56              |
| 34:BH:53:GLU:O    | 34:BH:54:ARG:HB3  | 2.06                     | 0.56              |
| 35:BI:10:GLU:O    | 35:BI:11:ASN:HB2  | 2.05                     | 0.56              |
| 37:BO:107:ARG:NH1 | 42:BT:36:GLU:H    | 2.04                     | 0.56              |
| 38:BP:115:LEU:HA  | 38:BP:134:ALA:CB  | 2.35                     | 0.56              |
| 39:BQ:27:VAL:HG11 | 39:BQ:134:ARG:HG2 | 1.87                     | 0.56              |
| 40:BR:21:TYR:HB3  | 40:BR:47:PHE:CE1  | 2.41                     | 0.56              |
| 40:BR:77:ARG:O    | 40:BR:81:ASP:OD2  | 2.23                     | 0.56              |
| 43:BU:41:ALA:O    | 43:BU:42:ALA:O    | 2.24                     | 0.56              |
| 1:CA:1288:A:O2'   | 1:CA:1289:A:H5'   | 2.06                     | 0.56              |
| 1:CA:1290:G:H3'   | 1:CA:1291:G:C8    | 2.41                     | 0.56              |
| 1:CA:944:G:H21    | 1:CA:1339:A:H62   | 1.53                     | 0.56              |
| 1:CA:52:G:C6      | 1:CA:360:A:C2     | 2.94                     | 0.56              |
| 1:CA:929:G:H2'    | 1:CA:930:C:H6     | 1.71                     | 0.56              |
| 2:CB:21:ARG:HB2   | 2:CB:38:GLY:O     | 2.06                     | 0.56              |
| 4:CD:60:GLU:OE1   | 4:CD:199:ASN:N    | 2.39                     | 0.56              |
| 9:CI:118:LYS:O    | 9:CI:120:ARG:N    | 2.38                     | 0.56              |
| 11:CK:74:ALA:C    | 11:CK:76:GLY:N    | 2.57                     | 0.56              |
| 13:CM:90:LEU:O    | 13:CM:91:ARG:CB   | 2.53                     | 0.56              |
| 15:CO:11:VAL:O    | 15:CO:14:GLU:HB3  | 2.06                     | 0.56              |
| 20:CT:10:LEU:O    | 20:CT:13:LEU:HD23 | 2.06                     | 0.56              |
| 23:CW:53:U:H4'    | 39:DQ:52:VAL:CG2  | 2.35                     | 0.56              |
| 24:CX:67:C:H2'    | 24:CX:67:C:O2     | 2.06                     | 0.56              |
| 49:D0:26:TYR:O    | 49:D0:29:GLN:HG3  | 2.06                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 55:D6:15:GLU:CG    | 55:D6:18:ARG:HE   | 2.17                     | 0.56              |
| 27:DA:1032:A:OP1   | 58:D9:8:LYS:HG2   | 2.05                     | 0.56              |
| 27:DA:1578:U:O2    | 27:DA:1578:U:H2'  | 2.05                     | 0.56              |
| 27:DA:1611:C:H5'   | 27:DA:1611:C:H6   | 1.70                     | 0.56              |
| 27:DA:1622:G:O2'   | 27:DA:1623:G:H5'  | 2.06                     | 0.56              |
| 27:DA:1799:G:H5'   | 27:DA:1819:A:H61  | 1.69                     | 0.56              |
| 27:DA:2050:C:C4    | 27:DA:2051:A:C2   | 2.93                     | 0.56              |
| 27:DA:267:C:H2'    | 27:DA:268:C:C6    | 2.39                     | 0.56              |
| 27:DA:542:C:N3     | 27:DA:543:C:N4    | 2.53                     | 0.56              |
| 27:DA:873:G:H4'    | 39:DQ:63:LYS:HE2  | 1.88                     | 0.56              |
| 28:DB:109:C:H5'    | 28:DB:110:G:O5'   | 2.05                     | 0.56              |
| 28:DB:26:A:H2'     | 28:DB:27:C:C6     | 2.40                     | 0.56              |
| 29:DC:45:ALA:O     | 29:DC:46:LYS:HB2  | 2.06                     | 0.56              |
| 29:DC:82:LYS:O     | 29:DC:83:ILE:HD13 | 2.06                     | 0.56              |
| 32:DF:20:LEU:HD22  | 32:DF:203:GLN:OE1 | 2.06                     | 0.56              |
| 38:DP:47:ASP:HB3   | 38:DP:48:PRO:O    | 2.05                     | 0.56              |
| 38:DP:50:ARG:HD3   | 57:D8:7:HIS:NE2   | 2.21                     | 0.56              |
| 43:DU:8:VAL:HG12   | 43:DU:12:ARG:HE   | 1.69                     | 0.56              |
| 43:DU:9:VAL:CG1    | 43:DU:13:LYS:HE3  | 2.35                     | 0.56              |
| 44:DV:4:ILE:O      | 44:DV:39:LEU:HD22 | 2.05                     | 0.56              |
| 46:DX:57:LEU:CD2   | 46:DX:78:LYS:HD3  | 2.35                     | 0.56              |
| 39:DQ:64:ILE:N     | 48:DZ:177:GLU:OE2 | 2.37                     | 0.56              |
| 1:AA:1415:G:O2'    | 1:AA:1416:G:H5'   | 2.06                     | 0.56              |
| 1:AA:1442:G:C8     | 1:AA:1442(B):A:C2 | 2.94                     | 0.56              |
| 1:AA:26:A:O2'      | 4:AD:209:ARG:NH2  | 2.39                     | 0.56              |
| 1:AA:841:U:H3'     | 1:AA:848:C:O4'    | 2.05                     | 0.56              |
| 2:AB:236:TYR:HA    | 2:AB:239:VAL:HG23 | 1.87                     | 0.56              |
| 3:AC:42:LEU:HA     | 3:AC:45:LYS:HD2   | 1.86                     | 0.56              |
| 8:AH:100:ILE:HB    | 8:AH:125:ARG:NH1  | 2.20                     | 0.56              |
| 8:AH:84:ARG:NH1    | 8:AH:84:ARG:CG    | 2.61                     | 0.56              |
| 11:AK:104:GLN:HE22 | 11:AK:106:LYS:HD2 | 1.70                     | 0.56              |
| 16:AP:14:ASN:OD1   | 16:AP:42:ARG:NH2  | 2.35                     | 0.56              |
| 16:AP:74:LEU:O     | 16:AP:79:VAL:HG23 | 2.06                     | 0.56              |
| 20:AT:63:ILE:CD1   | 20:AT:80:ARG:HB2  | 2.35                     | 0.56              |
| 25:AY:67:C:H2'     | 25:AY:68:C:H6     | 1.69                     | 0.56              |
| 51:B2:63:VAL:O     | 51:B2:66:GLU:HG2  | 2.06                     | 0.56              |
| 51:B2:7:ARG:HG3    | 51:B2:8:LYS:N     | 2.21                     | 0.56              |
| 27:BA:126:A:C6     | 27:BA:127:A:N1    | 2.74                     | 0.56              |
| 27:BA:2083:G:H2'   | 27:BA:2084:C:C6   | 2.41                     | 0.56              |
| 27:BA:2274:A:N1    | 27:BA:2276:G:H1'  | 2.20                     | 0.56              |
| 27:BA:2455:G:H2'   | 27:BA:2456:C:H6   | 1.70                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:226:G:H5''   | 27:BA:257:A:O2'    | 2.05                     | 0.56              |
| 27:BA:30:G:H2'     | 27:BA:31:C:H6      | 1.68                     | 0.56              |
| 27:BA:353:G:H2'    | 27:BA:354:G:H8     | 1.71                     | 0.56              |
| 27:BA:460:A:H3'    | 27:BA:461:C:H6     | 1.71                     | 0.56              |
| 27:BA:479:A:O2'    | 27:BA:481:G:H5'    | 2.06                     | 0.56              |
| 27:BA:844:C:H3'    | 27:BA:845:G:C8     | 2.40                     | 0.56              |
| 31:BE:117:MET:HB2  | 31:BE:122:PHE:O    | 2.06                     | 0.56              |
| 27:BA:2618:G:H21   | 31:BE:150:VAL:HG21 | 1.71                     | 0.56              |
| 31:BE:47:VAL:HG21  | 31:BE:86:PRO:HD3   | 1.87                     | 0.56              |
| 32:BF:2:LYS:HE2    | 32:BF:25:PRO:CB    | 2.31                     | 0.56              |
| 33:BG:114:ILE:O    | 33:BG:115:ARG:C    | 2.45                     | 0.56              |
| 34:BH:103:LEU:HD21 | 34:BH:105:LEU:HD22 | 1.88                     | 0.56              |
| 35:BI:139:GLN:O    | 35:BI:140:LEU:HB2  | 2.04                     | 0.56              |
| 37:BO:102:VAL:O    | 37:BO:122:LEU:O    | 2.23                     | 0.56              |
| 42:BT:35:LYS:C     | 42:BT:37:GLY:H     | 2.09                     | 0.56              |
| 42:BT:67:SER:O     | 42:BT:68:TYR:O     | 2.22                     | 0.56              |
| 45:BW:18:ARG:NH1   | 45:BW:76:VAL:O     | 2.38                     | 0.56              |
| 45:BW:92:ARG:O     | 45:BW:93:ALA:HB3   | 2.05                     | 0.56              |
| 47:BY:67:LEU:C     | 47:BY:67:LEU:HD12  | 2.25                     | 0.56              |
| 1:CA:1315:U:O2'    | 1:CA:1360:A:H1'    | 2.06                     | 0.56              |
| 1:CA:1347:G:C2     | 1:CA:1373:G:H2'    | 2.39                     | 0.56              |
| 1:CA:1498:U:H1'    | 1:CA:1499:A:N7     | 2.19                     | 0.56              |
| 1:CA:922:G:C6      | 1:CA:923:A:C6      | 2.93                     | 0.56              |
| 1:CA:929:G:H1      | 1:CA:1388:C:N4     | 2.03                     | 0.56              |
| 2:CB:24:TRP:CZ3    | 2:CB:26:PRO:HA     | 2.40                     | 0.56              |
| 3:CC:121:ALA:O     | 3:CC:125:GLU:HG3   | 2.06                     | 0.56              |
| 13:CM:23:TYR:HB3   | 13:CM:67:GLU:CB    | 2.34                     | 0.56              |
| 57:D8:61:LEU:O     | 57:D8:63:PRO:O     | 2.23                     | 0.56              |
| 27:DA:1348:G:H2'   | 27:DA:1349:A:H5''  | 1.87                     | 0.56              |
| 27:DA:143:G:C1'    | 46:DX:37:THR:HG21  | 2.36                     | 0.56              |
| 27:DA:1721:G:H5''  | 27:DA:1721:G:N3    | 2.21                     | 0.56              |
| 27:DA:1763:G:OP1   | 27:DA:1763:G:H4'   | 2.06                     | 0.56              |
| 27:DA:2258:C:O2'   | 27:DA:2426:A:H4'   | 2.06                     | 0.56              |
| 27:DA:2276:G:O2'   | 27:DA:2277:G:H8    | 1.88                     | 0.56              |
| 27:DA:2593:U:C2    | 27:DA:2594:C:H5    | 2.23                     | 0.56              |
| 27:DA:2607:G:H2'   | 27:DA:2608:G:O4'   | 2.06                     | 0.56              |
| 27:DA:428:A:H3'    | 27:DA:429:A:H8     | 1.70                     | 0.56              |
| 27:DA:479:A:O2'    | 27:DA:481:G:H5'    | 2.06                     | 0.56              |
| 27:DA:49:A:H1'     | 27:DA:51:G:C4      | 2.41                     | 0.56              |
| 27:DA:534:U:O2'    | 43:DU:49:HIS:HD2   | 1.89                     | 0.56              |
| 27:DA:570:G:O6     | 27:DA:2499:C:OP1   | 2.24                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:631:A:H2'    | 27:DA:632:A:O5'   | 2.06                     | 0.56              |
| 27:DA:941:A:O5'    | 38:DP:35:HIS:HE1  | 1.89                     | 0.56              |
| 30:DD:186:HIS:CD2  | 30:DD:188:GLU:HB2 | 2.39                     | 0.56              |
| 31:DE:67:PHE:HD2   | 31:DE:69:LYS:CE   | 2.19                     | 0.56              |
| 31:DE:91:VAL:HG12  | 31:DE:92:THR:N    | 2.21                     | 0.56              |
| 34:DH:104:GLU:CD   | 34:DH:112:PRO:HB2 | 2.26                     | 0.56              |
| 35:DI:92:VAL:CG1   | 35:DI:120:ILE:HB  | 2.35                     | 0.56              |
| 39:DQ:19:GLY:O     | 39:DQ:98:LYS:HD3  | 2.05                     | 0.56              |
| 40:DR:99:LYS:HZ3   | 54:D5:43:HIS:HB3  | 1.71                     | 0.56              |
| 41:DS:66:ALA:O     | 41:DS:69:VAL:CG1  | 2.53                     | 0.56              |
| 42:DT:132:LYS:C    | 42:DT:134:GLU:H   | 2.08                     | 0.56              |
| 46:DX:12:VAL:HG12  | 46:DX:27:THR:CB   | 2.36                     | 0.56              |
| 1:AA:1060:C:C5'    | 14:AN:45:ARG:HH22 | 2.18                     | 0.56              |
| 1:AA:129(A):G:N2   | 1:AA:189(E):U:H1' | 2.21                     | 0.56              |
| 1:AA:472:A:H2'     | 1:AA:473:G:O4'    | 2.05                     | 0.56              |
| 1:AA:538:G:H5''    | 12:AL:111:LYS:HB2 | 1.87                     | 0.56              |
| 1:AA:563:A:H5'     | 1:AA:566:G:N2     | 2.21                     | 0.56              |
| 5:AE:149:GLU:O     | 5:AE:151:LEU:N    | 2.39                     | 0.56              |
| 8:AH:9:MET:SD      | 8:AH:32:LYS:HD3   | 2.46                     | 0.56              |
| 13:AM:91:ARG:CB    | 13:AM:98:VAL:HG13 | 2.35                     | 0.56              |
| 14:AN:22:THR:O     | 14:AN:23:ARG:HB2  | 2.05                     | 0.56              |
| 18:AR:86:VAL:HG12  | 18:AR:87:ARG:CD   | 2.36                     | 0.56              |
| 27:BA:1848:A:H2'   | 27:BA:1849:G:H8   | 1.71                     | 0.56              |
| 27:BA:2161:C:H2'   | 27:BA:2162:G:C8   | 2.40                     | 0.56              |
| 27:BA:2425:A:H5''  | 27:BA:2427:C:O4'  | 2.05                     | 0.56              |
| 27:BA:814:C:OP1    | 44:BV:83:ARG:HA   | 2.06                     | 0.56              |
| 27:BA:83:G:N1      | 27:BA:102:G:O2'   | 2.37                     | 0.56              |
| 27:BA:839:U:O2'    | 27:BA:840:C:H5'   | 2.06                     | 0.56              |
| 27:BA:863:A:H2     | 27:BA:914:C:H41   | 1.54                     | 0.56              |
| 27:BA:271(K):U:O2' | 35:BI:50:ARG:HD3  | 2.05                     | 0.56              |
| 37:BO:78:ARG:CB    | 37:BO:78:ARG:NH1  | 2.69                     | 0.56              |
| 39:BQ:2:LEU:HG     | 39:BQ:70:PRO:HG3  | 1.88                     | 0.56              |
| 27:BA:1279:G:OP1   | 40:BR:35:THR:OG1  | 2.23                     | 0.56              |
| 44:BV:19:LYS:HZ1   | 44:BV:20:LEU:HB2  | 1.70                     | 0.56              |
| 45:BW:10:VAL:O     | 45:BW:10:VAL:HG12 | 2.06                     | 0.56              |
| 1:CA:1169:A:H2'    | 1:CA:1170:A:C8    | 2.41                     | 0.56              |
| 1:CA:1445:C:O2'    | 1:CA:1446:U:H5'   | 2.06                     | 0.56              |
| 1:CA:265:G:H4'     | 17:CQ:65:ILE:C    | 2.26                     | 0.56              |
| 1:CA:321:A:N6      | 1:CA:328:C:O2'    | 2.35                     | 0.56              |
| 2:CB:158:LEU:CD1   | 2:CB:158:LEU:H    | 2.03                     | 0.56              |
| 5:CE:29:GLY:HA2    | 5:CE:45:PHE:CE1   | 2.39                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CI:18:PHE:HD1    | 9:CI:62:TYR:HD2    | 1.54                     | 0.56              |
| 46:DX:60:ARG:NH2   | 56:D7:47:ARG:NH2   | 2.53                     | 0.56              |
| 57:D8:39:LYS:O     | 57:D8:42:ARG:HB3   | 2.06                     | 0.56              |
| 27:DA:631:A:OP2    | 57:D8:46:ARG:NH2   | 2.37                     | 0.56              |
| 27:DA:1146:C:HO2'  | 27:DA:1147:C:H5'   | 1.67                     | 0.56              |
| 27:DA:1388:G:H2'   | 27:DA:1389:G:H5'   | 1.87                     | 0.56              |
| 27:DA:1754:C:H5'   | 42:DT:101:PHE:CE2  | 2.41                     | 0.56              |
| 27:DA:1771:C:HO2'  | 27:DA:1786:A:H8    | 1.52                     | 0.56              |
| 27:DA:2443:C:O2'   | 27:DA:2444:G:H5'   | 2.06                     | 0.56              |
| 27:DA:2612:C:O2'   | 27:DA:2613:U:C5'   | 2.52                     | 0.56              |
| 27:DA:48:G:H5'     | 27:DA:52:A:C4'     | 2.35                     | 0.56              |
| 28:DB:26:A:C8      | 28:DB:26:A:H5''    | 2.41                     | 0.56              |
| 29:DC:78:ALA:CB    | 29:DC:82:LYS:HB2   | 2.35                     | 0.56              |
| 29:DC:87:GLU:HG2   | 29:DC:94:VAL:HG22  | 1.87                     | 0.56              |
| 30:DD:2:ALA:O      | 30:DD:3:VAL:CB     | 2.53                     | 0.56              |
| 31:DE:102:VAL:HG13 | 31:DE:172:VAL:HG23 | 1.88                     | 0.56              |
| 32:DF:53:THR:HG22  | 32:DF:56:GLU:HG3   | 1.87                     | 0.56              |
| 32:DF:65:TRP:CZ3   | 32:DF:73:ALA:O     | 2.58                     | 0.56              |
| 35:DI:133:HIS:CB   | 35:DI:134:PRO:CD   | 2.80                     | 0.56              |
| 32:DF:187:VAL:HB   | 38:DP:7:ARG:NH2    | 2.21                     | 0.56              |
| 40:DR:58:GLY:HA2   | 40:DR:80:PHE:HE1   | 1.71                     | 0.56              |
| 42:DT:92:GLY:C     | 42:DT:94:ALA:N     | 2.58                     | 0.56              |
| 44:DV:58:VAL:HG12  | 44:DV:59:ALA:H     | 1.71                     | 0.56              |
| 47:DY:95:LYS:HE2   | 47:DY:100:ALA:CB   | 2.35                     | 0.56              |
| 47:DY:26:LYS:HG2   | 47:DY:27:VAL:N     | 2.21                     | 0.56              |
| 47:DY:95:LYS:HE2   | 47:DY:100:ALA:HB2  | 1.88                     | 0.56              |
| 48:DZ:127:VAL:HG13 | 48:DZ:128:SER:N    | 2.21                     | 0.56              |
| 1:AA:1073:U:H2'    | 1:AA:1074:G:H8     | 1.70                     | 0.56              |
| 1:AA:1402:C:C2'    | 1:AA:1403:C:H5'    | 2.35                     | 0.56              |
| 1:AA:72:C:H2'      | 1:AA:73:G:H8       | 1.68                     | 0.56              |
| 1:AA:879:C:O2'     | 1:AA:880:C:H5'     | 2.06                     | 0.56              |
| 2:AB:24:TRP:N      | 2:AB:24:TRP:CD1    | 2.74                     | 0.56              |
| 3:AC:138:VAL:O     | 3:AC:138:VAL:HG12  | 2.06                     | 0.56              |
| 6:AF:40:VAL:HG23   | 6:AF:63:TYR:CE1    | 2.41                     | 0.56              |
| 1:AA:875:C:H1'     | 8:AH:15:ASN:HD21   | 1.71                     | 0.56              |
| 8:AH:93:VAL:O      | 8:AH:132:GLU:HA    | 2.06                     | 0.56              |
| 10:AJ:40:LEU:HG    | 10:AJ:69:ASN:HB3   | 1.88                     | 0.56              |
| 27:BA:1894:C:H6    | 27:BA:1894:C:O5'   | 1.89                     | 0.56              |
| 27:BA:271(J):C:H2' | 27:BA:271(J):C:O2  | 2.06                     | 0.56              |
| 32:BF:25:PRO:HG3   | 32:BF:119:ARG:CA   | 2.36                     | 0.56              |
| 38:BP:84:ASN:HD22  | 38:BP:115:LEU:CD2  | 2.18                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BR:8:ARG:CZ     | 40:BR:8:ARG:HA    | 2.36                     | 0.56              |
| 42:BT:65:LYS:NZ    | 42:BT:66:VAL:H    | 2.04                     | 0.56              |
| 42:BT:30:VAL:HG11  | 42:BT:84:GLN:HE22 | 1.71                     | 0.56              |
| 47:BY:80:GLY:O     | 47:BY:81:LYS:HB2  | 2.05                     | 0.56              |
| 1:CA:1306:A:N6     | 1:CA:1331:G:O2'   | 2.38                     | 0.56              |
| 1:CA:1452:C:O2'    | 1:CA:1456:G:N2    | 2.39                     | 0.56              |
| 1:CA:181:G:N2      | 1:CA:183:G:H22    | 2.04                     | 0.56              |
| 1:CA:486:U:HO2'    | 1:CA:487:A:H8     | 1.51                     | 0.56              |
| 1:CA:76:C:H42      | 1:CA:93:G:H1      | 1.54                     | 0.56              |
| 1:CA:773:G:H2'     | 1:CA:774:G:O4'    | 2.06                     | 0.56              |
| 1:CA:782:A:H2'     | 1:CA:783:C:O4'    | 2.06                     | 0.56              |
| 4:CD:33:MET:HE2    | 4:CD:33:MET:HA    | 1.87                     | 0.56              |
| 5:CE:48:ALA:HB1    | 5:CE:49:PRO:HD2   | 1.86                     | 0.56              |
| 7:CG:138:LYS:O     | 7:CG:141:VAL:HB   | 2.05                     | 0.56              |
| 8:CH:104:ARG:HB3   | 8:CH:107:LEU:HB2  | 1.87                     | 0.56              |
| 10:CJ:30:SER:HA    | 10:CJ:80:LYS:HD3  | 1.88                     | 0.56              |
| 19:CS:52:TYR:CE1   | 19:CS:56:GLN:HA   | 2.41                     | 0.56              |
| 27:DA:139(A):G:H22 | 46:DX:44:GLU:CD   | 2.09                     | 0.56              |
| 27:DA:1434:A:H2'   | 27:DA:1435:G:C8   | 2.41                     | 0.56              |
| 27:DA:1632:A:H8    | 27:DA:1632:A:O5'  | 1.89                     | 0.56              |
| 27:DA:2344:U:H4'   | 27:DA:2345:G:OP1  | 2.05                     | 0.56              |
| 27:DA:2525:G:H1    | 27:DA:2538:C:H42  | 1.54                     | 0.56              |
| 27:DA:2728:U:H5'   | 37:DO:70:LYS:NZ   | 2.21                     | 0.56              |
| 27:DA:2745:C:H4'   | 34:DH:142:GLY:C   | 2.25                     | 0.56              |
| 27:DA:587:C:C5     | 38:DP:33:ARG:NH1  | 2.74                     | 0.56              |
| 27:DA:612:C:H42    | 27:DA:615:G:H1    | 1.51                     | 0.56              |
| 27:DA:898:C:C2'    | 27:DA:899:A:H5'   | 2.35                     | 0.56              |
| 27:DA:820:A:C2     | 27:DA:943:U:H4'   | 2.41                     | 0.56              |
| 30:DD:9:TYR:CD2    | 30:DD:10:THR:HG22 | 2.41                     | 0.56              |
| 30:DD:45:ASN:OD1   | 30:DD:46:GLN:N    | 2.39                     | 0.56              |
| 31:DE:57:LYS:C     | 31:DE:59:VAL:H    | 2.10                     | 0.56              |
| 36:DN:126:PRO:O    | 36:DN:127:ASP:HB2 | 2.06                     | 0.56              |
| 27:DA:2416:C:OP1   | 38:DP:64:LYS:O    | 2.24                     | 0.56              |
| 42:DT:100:TYR:O    | 42:DT:103:ARG:HG3 | 2.06                     | 0.56              |
| 42:DT:22:PHE:N     | 42:DT:22:PHE:CD2  | 2.74                     | 0.56              |
| 45:DW:24:ILE:HG21  | 45:DW:36:LEU:HD11 | 1.87                     | 0.56              |
| 48:DZ:128:SER:C    | 48:DZ:130:ARG:H   | 2.09                     | 0.56              |
| 1:AA:1121:U:H6     | 1:AA:1121:U:O5'   | 1.89                     | 0.55              |
| 1:AA:1513:A:H2'    | 1:AA:1514:C:H6    | 1.68                     | 0.55              |
| 1:AA:24:U:O2'      | 1:AA:25:C:H5'     | 2.05                     | 0.55              |
| 1:AA:287:U:O2'     | 1:AA:288:A:H5'    | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:373:A:H5'    | 1:AA:373:A:H8     | 1.67                     | 0.55              |
| 1:AA:407:G:H1     | 1:AA:435:C:N4     | 2.04                     | 0.55              |
| 1:AA:974:A:OP2    | 14:AN:29:ARG:NH2  | 2.39                     | 0.55              |
| 3:AC:150:LYS:HB2  | 3:AC:173:VAL:HG21 | 1.89                     | 0.55              |
| 8:AH:124:ALA:HA   | 8:AH:129:VAL:HG22 | 1.87                     | 0.55              |
| 8:AH:5:PRO:O      | 8:AH:8:ASP:HB3    | 2.06                     | 0.55              |
| 9:AI:23:ASN:HB2   | 9:AI:60:ASP:OD2   | 2.05                     | 0.55              |
| 49:B0:73:GLY:O    | 49:B0:75:LEU:N    | 2.33                     | 0.55              |
| 55:B6:37:ARG:O    | 55:B6:48:VAL:O    | 2.22                     | 0.55              |
| 27:BA:1593:G:H2'  | 27:BA:1594:G:C8   | 2.41                     | 0.55              |
| 27:BA:1759:A:H5'' | 27:BA:2715:C:H1'  | 1.87                     | 0.55              |
| 27:BA:1876:A:H2'  | 27:BA:1877:A:C8   | 2.40                     | 0.55              |
| 27:BA:2369:A:O2'  | 27:BA:2370:G:H5'  | 2.06                     | 0.55              |
| 27:BA:2883:A:C5'  | 27:BA:2884:U:H5'  | 2.32                     | 0.55              |
| 27:BA:696:G:O2'   | 27:BA:697:C:H5'   | 2.06                     | 0.55              |
| 27:BA:752:A:O2'   | 27:BA:753:C:OP2   | 2.22                     | 0.55              |
| 27:BA:867:C:H2'   | 27:BA:868:U:H6    | 1.70                     | 0.55              |
| 30:BD:77:ALA:CB   | 30:BD:97:TYR:HA   | 2.36                     | 0.55              |
| 31:BE:152:LYS:HB3 | 36:BN:78:TYR:CD2  | 2.41                     | 0.55              |
| 31:BE:57:LYS:C    | 31:BE:59:VAL:N    | 2.57                     | 0.55              |
| 33:BG:170:ARG:HE  | 33:BG:174:GLU:CD  | 2.09                     | 0.55              |
| 33:BG:46:ALA:HA   | 33:BG:51:ARG:HB3  | 1.88                     | 0.55              |
| 38:BP:50:ARG:NH2  | 38:BP:50:ARG:HG2  | 2.21                     | 0.55              |
| 45:BW:23:LEU:O    | 45:BW:27:LYS:HD2  | 2.06                     | 0.55              |
| 1:CA:428:G:HO2'   | 1:CA:429:U:P      | 2.27                     | 0.55              |
| 1:CA:577:G:C4     | 1:CA:578:C:H5     | 2.24                     | 0.55              |
| 1:CA:893:C:H2'    | 1:CA:894:G:H8     | 1.70                     | 0.55              |
| 1:CA:977:A:O2'    | 1:CA:978:A:H5'    | 2.06                     | 0.55              |
| 2:CB:208:ILE:O    | 2:CB:208:ILE:HG22 | 2.06                     | 0.55              |
| 5:CE:80:ILE:O     | 5:CE:90:VAL:HA    | 2.06                     | 0.55              |
| 7:CG:155:ARG:O    | 7:CG:156:TRP:O    | 2.24                     | 0.55              |
| 10:CJ:63:PHE:HA   | 14:CN:59:ALA:CB   | 2.35                     | 0.55              |
| 12:CL:101:VAL:O   | 12:CL:102:TYR:HB2 | 2.04                     | 0.55              |
| 12:CL:30:ARG:O    | 12:CL:81:LEU:HD22 | 2.05                     | 0.55              |
| 13:CM:83:ASP:HB2  | 19:CS:66:MET:HE1  | 1.87                     | 0.55              |
| 13:CM:94:ARG:N    | 13:CM:94:ARG:HD2  | 2.21                     | 0.55              |
| 14:CN:26:ARG:HD2  | 14:CN:43:CYS:HB3  | 1.88                     | 0.55              |
| 18:CR:36:ASN:ND2  | 18:CR:36:ASN:N    | 2.53                     | 0.55              |
| 19:CS:24:ALA:O    | 19:CS:25:LYS:CB   | 2.53                     | 0.55              |
| 55:D6:14:THR:HA   | 55:D6:20:ASN:O    | 2.06                     | 0.55              |
| 27:DA:1907:G:C2   | 27:DA:1924:C:O2   | 2.58                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:2038:G:H2'  | 27:DA:2039:C:O4'   | 2.06                     | 0.55              |
| 27:DA:2066:C:C2'  | 27:DA:2067:G:O5'   | 2.54                     | 0.55              |
| 27:DA:2069:G:C6   | 27:DA:2443:C:N4    | 2.74                     | 0.55              |
| 27:DA:217:G:O6    | 27:DA:431:U:O2     | 2.24                     | 0.55              |
| 27:DA:2561:A:O2'  | 37:DO:40:VAL:HG21  | 2.05                     | 0.55              |
| 27:DA:2712:U:C2'  | 27:DA:2712(A):A:H8 | 2.19                     | 0.55              |
| 27:DA:436:C:H2'   | 27:DA:437:G:H8     | 1.71                     | 0.55              |
| 27:DA:65:C:H2'    | 27:DA:66:C:H6      | 1.71                     | 0.55              |
| 27:DA:732:C:N4    | 27:DA:733:G:C6     | 2.74                     | 0.55              |
| 29:DC:36:LYS:O    | 29:DC:37:PHE:C     | 2.44                     | 0.55              |
| 30:DD:13:ARG:HA   | 30:DD:16:MET:HB3   | 1.89                     | 0.55              |
| 31:DE:37:ARG:N    | 31:DE:46:ALA:O     | 2.35                     | 0.55              |
| 32:DF:118:ALA:C   | 32:DF:120:GLU:H    | 2.09                     | 0.55              |
| 33:DG:76:SER:HA   | 33:DG:83:ARG:CB    | 2.35                     | 0.55              |
| 34:DH:31:GLY:O    | 34:DH:79:VAL:HG12  | 2.07                     | 0.55              |
| 40:DR:41:ALA:C    | 40:DR:43:GLU:H     | 2.08                     | 0.55              |
| 42:DT:106:SER:HA  | 42:DT:110:ILE:HG13 | 1.88                     | 0.55              |
| 44:DV:46:VAL:HG13 | 44:DV:47:VAL:N     | 2.21                     | 0.55              |
| 44:DV:46:VAL:HG22 | 44:DV:47:VAL:H     | 1.71                     | 0.55              |
| 46:DX:64:LYS:NZ   | 46:DX:73:ARG:NH1   | 2.53                     | 0.55              |
| 47:DY:88:LYS:HD3  | 47:DY:93:GLY:N     | 2.21                     | 0.55              |
| 1:AA:359:U:H2'    | 1:AA:360:A:C8      | 2.41                     | 0.55              |
| 1:AA:434:U:H2'    | 1:AA:435:C:C1'     | 2.36                     | 0.55              |
| 1:AA:849:C:O2'    | 1:AA:850:U:H5'     | 2.05                     | 0.55              |
| 1:AA:981:U:H2'    | 1:AA:982:U:C5      | 2.40                     | 0.55              |
| 2:AB:91:PRO:CG    | 2:AB:155:LEU:HB2   | 2.36                     | 0.55              |
| 5:AE:84:PHE:HB2   | 5:AE:134:ALA:HB2   | 1.88                     | 0.55              |
| 9:AI:65:VAL:HG21  | 9:AI:73:GLN:HB3    | 1.88                     | 0.55              |
| 14:AN:42:ILE:HG22 | 14:AN:43:CYS:N     | 2.21                     | 0.55              |
| 25:AY:18:G:C4'    | 25:AY:56:G:H22     | 2.20                     | 0.55              |
| 50:B1:52:ARG:HG3  | 50:B1:53:VAL:N     | 2.19                     | 0.55              |
| 27:BA:2015:A:H1'  | 54:B5:2:ALA:HA     | 1.89                     | 0.55              |
| 27:BA:1474:C:H2'  | 27:BA:1475:G:C8    | 2.29                     | 0.55              |
| 27:BA:2091:U:O2'  | 50:B1:47:GLN:HG3   | 2.06                     | 0.55              |
| 27:BA:2110:G:OP2  | 27:BA:2110:G:C8    | 2.60                     | 0.55              |
| 27:BA:2328:A:H2'  | 27:BA:2329:G:C8    | 2.41                     | 0.55              |
| 27:BA:2555:U:C2'  | 27:BA:2556:C:H5'   | 2.36                     | 0.55              |
| 27:BA:444:C:O2'   | 27:BA:445:C:H5'    | 2.05                     | 0.55              |
| 27:BA:743:G:N2    | 27:BA:755:C:C2     | 2.75                     | 0.55              |
| 31:BE:104:VAL:O   | 31:BE:166:THR:HA   | 2.06                     | 0.55              |
| 33:BG:33:ARG:O    | 33:BG:162:THR:HG22 | 2.05                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BH:87:LEU:HD13  | 34:BH:162:ILE:HG21 | 1.88                     | 0.55              |
| 39:BQ:17:LEU:HD11  | 39:BQ:41:TRP:CD1   | 2.41                     | 0.55              |
| 40:BR:11:ASN:H     | 40:BR:17:ARG:HD3   | 1.71                     | 0.55              |
| 42:BT:115:ARG:O    | 42:BT:116:ALA:CB   | 2.55                     | 0.55              |
| 42:BT:127:ALA:C    | 42:BT:129:ARG:N    | 2.60                     | 0.55              |
| 42:BT:13:ARG:HA    | 42:BT:13:ARG:NE    | 2.17                     | 0.55              |
| 47:BY:37:VAL:HG23  | 47:BY:38:ILE:N     | 2.21                     | 0.55              |
| 48:BZ:110:VAL:HG13 | 48:BZ:110:VAL:O    | 2.06                     | 0.55              |
| 1:CA:1001(A):G:C8  | 1:CA:1002:G:H8     | 2.24                     | 0.55              |
| 1:CA:1027:C:H2'    | 1:CA:1028:C:C4     | 2.41                     | 0.55              |
| 1:CA:13:U:O2'      | 1:CA:14:U:H5''     | 2.06                     | 0.55              |
| 1:CA:72:C:O2'      | 1:CA:73:G:H5'      | 2.05                     | 0.55              |
| 1:CA:1074:G:H1'    | 2:CB:104:ASN:HD22  | 1.71                     | 0.55              |
| 1:CA:1104:G:H4'    | 2:CB:111:ARG:HH11  | 1.71                     | 0.55              |
| 2:CB:114:ARG:HA    | 2:CB:117:GLU:OE1   | 2.04                     | 0.55              |
| 5:CE:129:ILE:HG22  | 5:CE:130:ASN:N     | 2.21                     | 0.55              |
| 1:CA:1240:U:OP2    | 7:CG:116:ALA:HB2   | 2.06                     | 0.55              |
| 7:CG:27:ILE:HD13   | 7:CG:40:ALA:HA     | 1.87                     | 0.55              |
| 12:CL:21:VAL:HG22  | 12:CL:95:TYR:CZ    | 2.41                     | 0.55              |
| 12:CL:21:VAL:O     | 12:CL:23:ALA:N     | 2.37                     | 0.55              |
| 13:CM:76:ALA:HA    | 13:CM:79:LYS:CB    | 2.35                     | 0.55              |
| 13:CM:93:ARG:HB3   | 13:CM:94:ARG:HH11  | 1.72                     | 0.55              |
| 14:CN:2:ALA:O      | 14:CN:6:LEU:HD12   | 2.05                     | 0.55              |
| 19:CS:20:LEU:HA    | 19:CS:23:ASN:HB3   | 1.87                     | 0.55              |
| 19:CS:9:VAL:C      | 19:CS:11:VAL:H     | 2.10                     | 0.55              |
| 21:CU:8:THR:OG1    | 21:CU:11:GLY:HA3   | 2.05                     | 0.55              |
| 50:D1:59:THR:O     | 50:D1:91:LYS:NZ    | 2.34                     | 0.55              |
| 27:DA:1116:C:H2'   | 27:DA:1117:G:C8    | 2.41                     | 0.55              |
| 27:DA:118:A:H5'    | 27:DA:119:A:H8     | 1.69                     | 0.55              |
| 27:DA:1806:C:H2'   | 27:DA:1807:G:C8    | 2.42                     | 0.55              |
| 27:DA:1806:C:H2'   | 27:DA:1807:G:H8    | 1.71                     | 0.55              |
| 27:DA:2308:G:O6    | 27:DA:2310:A:N3    | 2.39                     | 0.55              |
| 27:DA:2538:C:H2'   | 27:DA:2539:C:H6    | 1.72                     | 0.55              |
| 27:DA:2594:C:O2'   | 27:DA:2595:G:H5'   | 2.07                     | 0.55              |
| 27:DA:752:A:O2'    | 27:DA:753:C:OP2    | 2.23                     | 0.55              |
| 27:DA:820:A:N3     | 27:DA:943:U:H4'    | 2.20                     | 0.55              |
| 29:DC:20:TYR:HD1   | 29:DC:20:TYR:H     | 1.54                     | 0.55              |
| 31:DE:1:MET:HG3    | 31:DE:200:GLU:OE1  | 2.06                     | 0.55              |
| 32:DF:22:ALA:C     | 32:DF:24:LEU:N     | 2.58                     | 0.55              |
| 34:DH:137:ASP:CB   | 34:DH:140:LYS:HB3  | 2.36                     | 0.55              |
| 35:DI:7:GLU:HG3    | 35:DI:8:PRO:HD2    | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DN:2:LYS:HB3   | 36:DN:4:TYR:CE2   | 2.42                     | 0.55              |
| 31:DE:110:GLY:O   | 40:DR:2:ARG:NE    | 2.39                     | 0.55              |
| 40:DR:55:ALA:HA   | 40:DR:80:PHE:CZ   | 2.41                     | 0.55              |
| 41:DS:25:ARG:HH12 | 41:DS:40:ILE:HD12 | 1.71                     | 0.55              |
| 48:DZ:150:HIS:HB3 | 48:DZ:169:THR:CA  | 2.37                     | 0.55              |
| 1:AA:113:G:H21    | 1:AA:353:A:H1'    | 1.71                     | 0.55              |
| 1:AA:1349:A:OP2   | 9:AI:118:LYS:NZ   | 2.38                     | 0.55              |
| 1:AA:1402:C:H2'   | 1:AA:1403:C:O4'   | 2.06                     | 0.55              |
| 1:AA:1510:U:H2'   | 1:AA:1511:G:H8    | 1.67                     | 0.55              |
| 1:AA:324:G:C8     | 1:AA:324:G:C3'    | 2.90                     | 0.55              |
| 1:AA:452:A:O2'    | 1:AA:453:A:H8     | 1.79                     | 0.55              |
| 1:AA:614:A:C2     | 1:AA:615:C:C2     | 2.94                     | 0.55              |
| 8:AH:67:PRO:C     | 8:AH:76:PRO:HB3   | 2.26                     | 0.55              |
| 8:AH:74:PRO:HG2   | 8:AH:75:ARG:N     | 2.22                     | 0.55              |
| 50:B1:20:ARG:HA   | 50:B1:33:LYS:O    | 2.05                     | 0.55              |
| 27:BA:686:G:C2    | 56:B7:11:LYS:HE3  | 2.40                     | 0.55              |
| 27:BA:1490:A:C2   | 30:BD:75:ILE:HG23 | 2.41                     | 0.55              |
| 27:BA:2127:G:O2'  | 27:BA:2128:C:C6   | 2.53                     | 0.55              |
| 27:BA:2126:A:N6   | 27:BA:2163:C:H5'  | 2.21                     | 0.55              |
| 27:BA:2230:G:H4'  | 50:B1:43:TYR:HB2  | 1.88                     | 0.55              |
| 27:BA:90:U:C2'    | 27:BA:90:U:O2     | 2.51                     | 0.55              |
| 32:BF:65:TRP:CB   | 32:BF:66:PRO:CD   | 2.85                     | 0.55              |
| 37:BO:40:VAL:HG13 | 37:BO:57:VAL:HG12 | 1.87                     | 0.55              |
| 37:BO:66:LYS:HA   | 37:BO:79:PHE:O    | 2.07                     | 0.55              |
| 40:BR:118:GLU:HA  | 40:BR:118:GLU:OE1 | 2.05                     | 0.55              |
| 40:BR:11:ASN:OD1  | 40:BR:11:ASN:O    | 2.23                     | 0.55              |
| 40:BR:79:LEU:O    | 40:BR:83:ILE:HB   | 2.06                     | 0.55              |
| 44:BV:46:VAL:HG13 | 44:BV:47:VAL:N    | 2.21                     | 0.55              |
| 45:BW:31:GLU:O    | 45:BW:35:ILE:HG13 | 2.06                     | 0.55              |
| 46:BX:84:ALA:O    | 46:BX:87:GLN:HG3  | 2.06                     | 0.55              |
| 47:BY:62:GLU:OE1  | 47:BY:62:GLU:HA   | 2.06                     | 0.55              |
| 47:BY:67:LEU:O    | 47:BY:68:HIS:O    | 2.24                     | 0.55              |
| 1:CA:1311:G:C6    | 1:CA:1312:G:N7    | 2.75                     | 0.55              |
| 1:CA:455:C:O2'    | 1:CA:456:C:H5'    | 2.06                     | 0.55              |
| 1:CA:578:C:O2     | 1:CA:579:G:C8     | 2.59                     | 0.55              |
| 1:CA:929:G:H2'    | 1:CA:930:C:C6     | 2.41                     | 0.55              |
| 3:CC:181:ASN:O    | 3:CC:204:LEU:HB2  | 2.06                     | 0.55              |
| 11:CK:115:PRO:C   | 11:CK:117:ASN:H   | 2.10                     | 0.55              |
| 11:CK:125:PHE:N   | 11:CK:125:PHE:CD1 | 2.74                     | 0.55              |
| 16:CP:5:ARG:NH1   | 16:CP:24:ALA:HA   | 2.17                     | 0.55              |
| 18:CR:70:ILE:HG22 | 18:CR:74:ARG:HD2  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:CU:24:ARG:O    | 21:CU:25:LYS:CB    | 2.53                     | 0.55              |
| 22:CV:7:C:H2'     | 22:CV:8:A:H8       | 1.71                     | 0.55              |
| 23:CW:18:G:H4'    | 23:CW:19:U:O4'     | 2.07                     | 0.55              |
| 52:D3:26:LEU:HD21 | 52:D3:46:ASN:HB2   | 1.89                     | 0.55              |
| 27:DA:1158:C:HO2' | 27:DA:1159:U:H6    | 1.50                     | 0.55              |
| 27:DA:1441:G:H2'  | 27:DA:1442:G:H8    | 1.70                     | 0.55              |
| 27:DA:1702:G:H2'  | 27:DA:1703:G:O4'   | 2.06                     | 0.55              |
| 27:DA:17:G:H4'    | 43:DU:25:TRP:CZ3   | 2.41                     | 0.55              |
| 27:DA:1961:C:O2'  | 27:DA:1962:C:H5'   | 2.07                     | 0.55              |
| 27:DA:2377:A:H2'  | 27:DA:2378:A:C8    | 2.41                     | 0.55              |
| 27:DA:2539:C:N3   | 27:DA:2540:C:C5    | 2.75                     | 0.55              |
| 27:DA:2581:G:H8   | 27:DA:2582:G:O6    | 1.89                     | 0.55              |
| 27:DA:2616:C:H2'  | 27:DA:2617:C:C6    | 2.41                     | 0.55              |
| 27:DA:2831:G:P    | 31:DE:58:ARG:HH22  | 2.29                     | 0.55              |
| 27:DA:319:C:C2    | 27:DA:320:A:C8     | 2.94                     | 0.55              |
| 27:DA:435:C:O2'   | 27:DA:436:C:H5'    | 2.06                     | 0.55              |
| 27:DA:673:C:O2'   | 27:DA:674:G:H5'    | 2.06                     | 0.55              |
| 27:DA:914:C:N4    | 27:DA:915:C:C2     | 2.74                     | 0.55              |
| 27:DA:975(A):G:N2 | 27:DA:976:C:H1'    | 2.20                     | 0.55              |
| 27:DA:97:C:C2     | 27:DA:98:G:C8      | 2.94                     | 0.55              |
| 32:DF:78:ILE:HA   | 32:DF:83:PHE:CE1   | 2.41                     | 0.55              |
| 34:DH:104:GLU:OE2 | 34:DH:112:PRO:HB2  | 2.06                     | 0.55              |
| 35:DI:29:TYR:HD2  | 35:DI:30:LEU:HG    | 1.71                     | 0.55              |
| 27:DA:626:U:H3    | 38:DP:105:LEU:CB   | 2.19                     | 0.55              |
| 38:DP:16:ARG:NH1  | 38:DP:16:ARG:HB2   | 2.20                     | 0.55              |
| 40:DR:28:LEU:HD12 | 40:DR:48:VAL:HG21  | 1.88                     | 0.55              |
| 42:DT:129:ARG:CZ  | 42:DT:131:ALA:HB3  | 2.36                     | 0.55              |
| 42:DT:89:VAL:O    | 42:DT:91:ARG:HG3   | 2.06                     | 0.55              |
| 45:DW:65:LEU:HD23 | 45:DW:67:ASP:H     | 1.71                     | 0.55              |
| 46:DX:5:TYR:HE2   | 51:D2:30:ARG:HE    | 1.54                     | 0.55              |
| 1:AA:1064:G:O2'   | 1:AA:1065:U:O5'    | 2.21                     | 0.55              |
| 1:AA:1086:U:H6    | 1:AA:1086:U:H5'    | 1.72                     | 0.55              |
| 1:AA:1155:G:O2'   | 1:AA:1156:G:H5'    | 2.06                     | 0.55              |
| 1:AA:1525:G:P     | 11:AK:120:ARG:HH22 | 2.29                     | 0.55              |
| 1:AA:324:G:OP1    | 20:AT:70:SER:HB2   | 2.06                     | 0.55              |
| 1:AA:372:C:H4'    | 1:AA:373:A:OP1     | 2.06                     | 0.55              |
| 1:AA:471:G:C2'    | 1:AA:472:A:H8      | 2.19                     | 0.55              |
| 1:AA:68:G:C2      | 1:AA:69:G:H1'      | 2.42                     | 0.55              |
| 1:AA:953:G:H2'    | 1:AA:954:G:O4'     | 2.07                     | 0.55              |
| 8:AH:87:SER:HB3   | 8:AH:133:LEU:O     | 2.06                     | 0.55              |
| 8:AH:81:HIS:HB2   | 8:AH:138:TRP:CZ3   | 2.41                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:AM:67:GLU:OE2  | 13:AM:71:ARG:NH2   | 2.39                     | 0.55              |
| 27:BA:2330:G:H21  | 49:B0:42:GLY:HA2   | 1.71                     | 0.55              |
| 58:B9:24:TYR:CD2  | 58:B9:35:ARG:HG3   | 2.41                     | 0.55              |
| 27:BA:1346:G:C5   | 27:BA:1347:G:N7    | 2.75                     | 0.55              |
| 27:BA:1368:G:C2   | 27:BA:1369:G:C8    | 2.95                     | 0.55              |
| 27:BA:1999:C:C2   | 27:BA:2000:G:C8    | 2.94                     | 0.55              |
| 27:BA:2416:C:C6   | 27:BA:2416:C:O5'   | 2.58                     | 0.55              |
| 27:BA:782:A:C5'   | 27:BA:783:A:C2     | 2.90                     | 0.55              |
| 29:BC:68:LEU:O    | 29:BC:69:GLY:C     | 2.45                     | 0.55              |
| 32:BF:82:ILE:O    | 32:BF:82:ILE:CG1   | 2.54                     | 0.55              |
| 33:BG:56:ALA:HB2  | 33:BG:153:ARG:NH2  | 2.22                     | 0.55              |
| 34:BH:103:LEU:HB3 | 34:BH:123:PHE:CD2  | 2.42                     | 0.55              |
| 34:BH:19:VAL:CB   | 34:BH:44:VAL:HG13  | 2.36                     | 0.55              |
| 35:BI:11:ASN:O    | 35:BI:12:LEU:HB3   | 2.05                     | 0.55              |
| 38:BP:95:VAL:CG2  | 38:BP:125:VAL:HG12 | 2.32                     | 0.55              |
| 38:BP:50:ARG:HG3  | 38:BP:51:PHE:N     | 2.20                     | 0.55              |
| 40:BR:33:ARG:HE   | 40:BR:115:GLU:HB2  | 1.72                     | 0.55              |
| 40:BR:18:LEU:CD1  | 40:BR:22:ARG:CZ    | 2.84                     | 0.55              |
| 41:BS:48:LEU:O    | 41:BS:49:VAL:CG2   | 2.52                     | 0.55              |
| 37:BO:64:ARG:HD2  | 42:BT:70:VAL:HG11  | 1.87                     | 0.55              |
| 48:BZ:143:LEU:HB3 | 48:BZ:147:ASP:O    | 2.06                     | 0.55              |
| 1:CA:1321:C:C6    | 1:CA:1322:C:H2'    | 2.41                     | 0.55              |
| 1:CA:1338:G:H2'   | 1:CA:1339:A:H8     | 1.68                     | 0.55              |
| 1:CA:252:U:C2     | 1:CA:253:U:C5      | 2.95                     | 0.55              |
| 1:CA:472:A:H4'    | 16:CP:82:GLN:NE2   | 2.20                     | 0.55              |
| 1:CA:583:A:H1'    | 1:CA:759:A:N6      | 2.22                     | 0.55              |
| 1:CA:697:U:H3'    | 1:CA:698:G:H8      | 1.71                     | 0.55              |
| 1:CA:737:A:H2'    | 1:CA:738:C:C6      | 2.41                     | 0.55              |
| 2:CB:180:LEU:O    | 2:CB:182:ILE:HG13  | 2.06                     | 0.55              |
| 4:CD:130:GLY:O    | 4:CD:131:ARG:C     | 2.44                     | 0.55              |
| 4:CD:187:ARG:HH11 | 4:CD:187:ARG:HG2   | 1.71                     | 0.55              |
| 7:CG:86:GLN:NE2   | 25:CY:30:A:C2      | 2.73                     | 0.55              |
| 10:CJ:81:THR:O    | 10:CJ:85:LEU:HG    | 2.05                     | 0.55              |
| 11:CK:48:ILE:HD11 | 11:CK:64:ALA:HA    | 1.86                     | 0.55              |
| 12:CL:3:THR:C     | 12:CL:7:LEU:HD12   | 2.27                     | 0.55              |
| 1:CA:750:G:H1'    | 15:CO:22:THR:OG1   | 2.05                     | 0.55              |
| 1:CA:667:G:O2'    | 15:CO:49:ASP:OD1   | 2.14                     | 0.55              |
| 17:CQ:7:THR:C     | 17:CQ:23:VAL:HG13  | 2.27                     | 0.55              |
| 20:CT:26:ASN:HD22 | 20:CT:27:LYS:N     | 2.04                     | 0.55              |
| 1:CA:263:A:OP1    | 20:CT:79:ARG:HD2   | 2.05                     | 0.55              |
| 20:CT:8:ARG:HH11  | 20:CT:8:ARG:HG3    | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:D2:21:LEU:O    | 51:D2:25:VAL:HG23 | 2.06                     | 0.55              |
| 27:DA:1162:G:C2'  | 27:DA:1163:G:H5'  | 2.36                     | 0.55              |
| 27:DA:1569:A:C2'  | 30:DD:38:LYS:HZ3  | 2.18                     | 0.55              |
| 27:DA:1996:C:H4'  | 27:DA:1997:G:OP1  | 2.07                     | 0.55              |
| 27:DA:2292:C:O2'  | 27:DA:2293:C:H5'  | 2.06                     | 0.55              |
| 27:DA:2405:G:O2'  | 27:DA:2411:A:N6   | 2.40                     | 0.55              |
| 27:DA:2251:G:C8   | 27:DA:2450:A:H4'  | 2.41                     | 0.55              |
| 27:DA:2646:C:H2'  | 27:DA:2647:U:O4'  | 2.07                     | 0.55              |
| 27:DA:265:A:N7    | 27:DA:283:A:N6    | 2.53                     | 0.55              |
| 27:DA:357:A:H2'   | 27:DA:358:U:O4'   | 2.07                     | 0.55              |
| 27:DA:661:C:H2'   | 27:DA:662:G:H8    | 1.70                     | 0.55              |
| 27:DA:686:G:H5''  | 56:D7:11:LYS:HE2  | 1.87                     | 0.55              |
| 27:DA:71:A:H5'    | 27:DA:71:A:H8     | 1.72                     | 0.55              |
| 27:DA:946:G:C2    | 27:DA:947:G:C4    | 2.95                     | 0.55              |
| 30:DD:43:ARG:HB2  | 30:DD:54:ARG:HB3  | 1.87                     | 0.55              |
| 30:DD:44:ASN:HB2  | 30:DD:48:ARG:O    | 2.07                     | 0.55              |
| 31:DE:69:LYS:O    | 31:DE:71:GLY:N    | 2.39                     | 0.55              |
| 32:DF:33:LEU:HD11 | 32:DF:109:GLY:CA  | 2.36                     | 0.55              |
| 33:DG:98:ARG:HA   | 33:DG:101:ILE:CG2 | 2.36                     | 0.55              |
| 35:DI:7:GLU:CD    | 35:DI:8:PRO:HD2   | 2.27                     | 0.55              |
| 39:DQ:135:ASP:OD1 | 39:DQ:135:ASP:N   | 2.38                     | 0.55              |
| 27:DA:2880:C:HO2' | 40:DR:90:ARG:HD3  | 1.71                     | 0.55              |
| 44:DV:1:MET:HA    | 44:DV:1:MET:HE2   | 1.88                     | 0.55              |
| 1:AA:1075:C:H4'   | 1:AA:1101:A:N6    | 2.22                     | 0.55              |
| 1:AA:259:G:H2'    | 1:AA:260:G:H8     | 1.70                     | 0.55              |
| 1:AA:587:G:O2'    | 1:AA:588:G:H5'    | 2.07                     | 0.55              |
| 2:AB:53:ARG:CZ    | 2:AB:199:TYR:HE2  | 2.18                     | 0.55              |
| 3:AC:132:ARG:O    | 3:AC:136:GLN:HB2  | 2.07                     | 0.55              |
| 5:AE:28:PHE:O     | 5:AE:47:LYS:HA    | 2.07                     | 0.55              |
| 7:AG:152:ALA:O    | 7:AG:155:ARG:NH1  | 2.39                     | 0.55              |
| 17:AQ:9:VAL:O     | 17:AQ:22:LEU:N    | 2.37                     | 0.55              |
| 24:AX:25:C:H2'    | 24:AX:26:G:H8     | 1.71                     | 0.55              |
| 51:B2:47:ASN:O    | 51:B2:50:ILE:HG13 | 2.06                     | 0.55              |
| 55:B6:33:LYS:CA   | 55:B6:33:LYS:HE2  | 2.34                     | 0.55              |
| 57:B8:30:ARG:HA   | 57:B8:30:ARG:NE   | 2.21                     | 0.55              |
| 27:BA:1020:A:C4'  | 27:BA:1021:A:O5'  | 2.45                     | 0.55              |
| 27:BA:1431:U:O2'  | 27:BA:1432:C:H5'  | 2.06                     | 0.55              |
| 27:BA:1721:G:C2   | 27:BA:1739:U:OP2  | 2.59                     | 0.55              |
| 27:BA:2162:G:H4'  | 27:BA:2172:U:HO2' | 1.69                     | 0.55              |
| 27:BA:2183:C:H2'  | 27:BA:2184:G:C8   | 2.38                     | 0.55              |
| 27:BA:2292:C:O2'  | 27:BA:2293:C:H5'  | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:237:C:H2'    | 27:BA:238:C:H6     | 1.71                     | 0.55              |
| 27:BA:81:G:N2      | 27:BA:106:C:C2     | 2.73                     | 0.55              |
| 28:BB:45:A:C2      | 28:BB:46:A:H1'     | 2.42                     | 0.55              |
| 32:BF:36:VAL:O     | 32:BF:39:TRP:HB3   | 2.07                     | 0.55              |
| 35:BI:121:LYS:O    | 35:BI:122:GLU:HB2  | 2.05                     | 0.55              |
| 35:BI:29:TYR:CD1   | 35:BI:33:ARG:NE    | 2.75                     | 0.55              |
| 27:BA:2393:A:H5'   | 38:BP:62:LEU:HB3   | 1.89                     | 0.55              |
| 27:BA:956:G:H5''   | 39:BQ:77:LYS:HD2   | 1.87                     | 0.55              |
| 43:BU:21:ALA:HB1   | 43:BU:24:TYR:CD1   | 2.42                     | 0.55              |
| 36:BN:4:TYR:HB2    | 43:BU:64:ARG:CZ    | 2.37                     | 0.55              |
| 1:CA:177:C:O2'     | 1:CA:178:C:H5'     | 2.07                     | 0.55              |
| 2:CB:70:PHE:CD2    | 2:CB:163:PHE:HB3   | 2.42                     | 0.55              |
| 4:CD:185:PHE:HD2   | 4:CD:185:PHE:O     | 1.90                     | 0.55              |
| 8:CH:109:ILE:HG12  | 8:CH:110:ALA:N     | 2.15                     | 0.55              |
| 10:CJ:28:ARG:NH1   | 10:CJ:33:GLN:HA    | 2.22                     | 0.55              |
| 52:D3:13:ILE:H     | 52:D3:13:ILE:HD12  | 1.71                     | 0.55              |
| 27:DA:2285:C:OP2   | 55:D6:27:LYS:HD2   | 2.07                     | 0.55              |
| 27:DA:1042:G:H3'   | 27:DA:1043:C:O4'   | 2.06                     | 0.55              |
| 27:DA:1164:G:C6    | 27:DA:1165:U:C4    | 2.95                     | 0.55              |
| 27:DA:1362:C:O2'   | 27:DA:1363:C:H5'   | 2.07                     | 0.55              |
| 27:DA:1577:C:H2'   | 27:DA:1578:U:C6    | 2.42                     | 0.55              |
| 27:DA:2031:A:O2'   | 27:DA:2032:G:P     | 2.63                     | 0.55              |
| 27:DA:2084:C:O2'   | 27:DA:2085:C:H5'   | 2.06                     | 0.55              |
| 27:DA:2122:U:H2'   | 27:DA:2123:G:C8    | 2.41                     | 0.55              |
| 27:DA:2107:C:N4    | 27:DA:2182:G:H1    | 1.94                     | 0.55              |
| 27:DA:2302:G:H21   | 33:DG:128:ARG:HD2  | 1.72                     | 0.55              |
| 27:DA:2619:C:H4'   | 31:DE:150:VAL:HG12 | 1.87                     | 0.55              |
| 27:DA:283:A:N1     | 27:DA:427:U:H1'    | 2.20                     | 0.55              |
| 27:DA:941:A:P      | 38:DP:35:HIS:HE1   | 2.29                     | 0.55              |
| 30:DD:30:GLU:OE1   | 30:DD:84:TYR:O     | 2.24                     | 0.55              |
| 30:DD:71:ASP:CB    | 30:DD:103:ARG:HH22 | 2.20                     | 0.55              |
| 34:DH:149:ARG:HH21 | 34:DH:154:PRO:CG   | 2.18                     | 0.55              |
| 35:DI:101:LEU:HD12 | 35:DI:105:HIS:HB2  | 1.88                     | 0.55              |
| 41:DS:89:ARG:C     | 41:DS:92:TYR:HB3   | 2.27                     | 0.55              |
| 42:DT:129:ARG:HD2  | 42:DT:131:ALA:HB3  | 1.87                     | 0.55              |
| 43:DU:92:ARG:NH1   | 43:DU:92:ARG:CG    | 2.66                     | 0.55              |
| 44:DV:64:HIS:ND1   | 44:DV:92:THR:CG2   | 2.69                     | 0.55              |
| 44:DV:77:ALA:O     | 44:DV:79:VAL:HG12  | 2.05                     | 0.55              |
| 45:DW:20:VAL:C     | 45:DW:22:ASP:H     | 2.10                     | 0.55              |
| 45:DW:62:HIS:O     | 45:DW:64:MET:HG3   | 2.06                     | 0.55              |
| 47:DY:9:LYS:C      | 47:DY:11:ASP:H     | 2.10                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:DZ:19:ARG:C     | 48:DZ:21:GLY:H     | 2.08                     | 0.55              |
| 48:DZ:55:VAL:HG12  | 48:DZ:56:ILE:N     | 2.20                     | 0.55              |
| 48:DZ:60:LEU:CG    | 48:DZ:64:GLN:HB2   | 2.37                     | 0.55              |
| 2:AB:105:PHE:HZ    | 2:AB:155:LEU:O     | 1.90                     | 0.55              |
| 2:AB:178:ARG:NH1   | 2:AB:178:ARG:HG2   | 2.21                     | 0.55              |
| 2:AB:87:ARG:NH1    | 2:AB:220:ASP:OD1   | 2.37                     | 0.55              |
| 7:AG:15:ASP:CB     | 7:AG:20:ASP:H      | 2.19                     | 0.55              |
| 11:AK:114:VAL:HG13 | 11:AK:114:VAL:O    | 2.07                     | 0.55              |
| 11:AK:21:ILE:N     | 11:AK:21:ILE:HD12  | 2.21                     | 0.55              |
| 12:AL:22:PRO:HD2   | 12:AL:94:ARG:NH2   | 2.21                     | 0.55              |
| 12:AL:79:VAL:C     | 12:AL:80:VAL:HG22  | 2.27                     | 0.55              |
| 10:AJ:49:VAL:HG23  | 14:AN:41:ARG:HB2   | 1.88                     | 0.55              |
| 15:AO:31:LEU:HG    | 15:AO:31:LEU:O     | 2.07                     | 0.55              |
| 18:AR:26:LEU:HG    | 18:AR:42:ARG:NH1   | 2.21                     | 0.55              |
| 20:AT:12:ALA:C     | 20:AT:14:LYS:N     | 2.56                     | 0.55              |
| 20:AT:28:ALA:O     | 20:AT:30:LYS:N     | 2.39                     | 0.55              |
| 23:AW:68:C:H2'     | 23:AW:68:C:O2      | 2.05                     | 0.55              |
| 25:AY:18:G:H22     | 25:AY:55:C:N4      | 2.05                     | 0.55              |
| 51:B2:21:LEU:HD13  | 51:B2:64:LEU:HA    | 1.87                     | 0.55              |
| 55:B6:16:CYS:SG    | 55:B6:48:VAL:CG2   | 2.95                     | 0.55              |
| 27:BA:1280:G:C2    | 27:BA:1281:G:H1'   | 2.41                     | 0.55              |
| 27:BA:1598:C:H5'   | 46:BX:36:LYS:CB    | 2.36                     | 0.55              |
| 27:BA:1848:A:O2'   | 27:BA:1849:G:O5'   | 2.24                     | 0.55              |
| 27:BA:2048:G:C2'   | 27:BA:2049:G:O5'   | 2.54                     | 0.55              |
| 27:BA:2307:G:N2    | 27:BA:2308:G:H5''  | 2.22                     | 0.55              |
| 27:BA:363(F):A:O2' | 27:BA:364:C:H5     | 1.90                     | 0.55              |
| 27:BA:414:C:H3'    | 27:BA:415:A:H8     | 1.71                     | 0.55              |
| 27:BA:224:G:O6     | 27:BA:420:C:H5'    | 2.07                     | 0.55              |
| 27:BA:748:G:H2'    | 27:BA:750:A:N7     | 2.22                     | 0.55              |
| 27:BA:977:G:C2'    | 27:BA:978:G:H5'    | 2.37                     | 0.55              |
| 30:BD:129:ASN:O    | 30:BD:193:VAL:HG12 | 2.06                     | 0.55              |
| 33:BG:91:ARG:C     | 33:BG:91:ARG:CD    | 2.75                     | 0.55              |
| 35:BI:42:SER:C     | 35:BI:44:LEU:H     | 2.10                     | 0.55              |
| 40:BR:109:ALA:O    | 40:BR:111:LEU:HD22 | 2.06                     | 0.55              |
| 41:BS:34:HIS:CD2   | 41:BS:53:SER:HB3   | 2.42                     | 0.55              |
| 43:BU:92:ARG:HG2   | 44:BV:11:GLN:OE1   | 2.07                     | 0.55              |
| 46:BX:12:VAL:CB    | 46:BX:17:ALA:HB1   | 2.37                     | 0.55              |
| 47:BY:95:LYS:NZ    | 47:BY:99:CYS:O     | 2.31                     | 0.55              |
| 1:CA:1142:G:H2'    | 1:CA:1143:G:C8     | 2.41                     | 0.55              |
| 1:CA:1294:G:H2'    | 1:CA:1295:G:C8     | 2.42                     | 0.55              |
| 1:CA:1486:G:H2'    | 1:CA:1487:G:C8     | 2.42                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CA:686:U:O2    | 1:CA:687:A:N7     | 2.40                     | 0.55              |
| 1:CA:818:G:O2'   | 1:CA:819:A:H5''   | 2.07                     | 0.55              |
| 4:CD:193:ASP:OD1 | 4:CD:193:ASP:N    | 2.38                     | 0.55              |
| 2:CB:178:ARG:NH2 | 8:CH:74:PRO:HG3   | 2.21                     | 0.55              |
| 12:CL:66:TYR:HD2 | 12:CL:67:ILE:H    | 1.54                     | 0.55              |
| 16:CP:76:GLN:HG2 | 16:CP:76:GLN:O    | 2.05                     | 0.55              |
| 6:CF:97:PHE:O    | 18:CR:31:LEU:HD23 | 2.06                     | 0.55              |
| 20:CT:16:HIS:HA  | 20:CT:19:SER:CB   | 2.37                     | 0.55              |
| 51:D2:18:PRO:HG2 | 51:D2:19:VAL:HG23 | 1.87                     | 0.55              |
| 56:D7:8:ASN:ND2  | 56:D7:8:ASN:C     | 2.59                     | 0.55              |
| 27:DA:1497:U:O4' | 27:DA:1497:U:OP1  | 2.25                     | 0.55              |
| 27:DA:1659:U:O2' | 27:DA:1660:C:H5'  | 2.07                     | 0.55              |
| 27:DA:392:C:H5'' | 27:DA:409:C:H5''  | 1.89                     | 0.55              |
| 27:DA:74:A:H4'   | 27:DA:75:G:O5'    | 2.07                     | 0.55              |
| 28:DB:35:U:O2'   | 28:DB:36:C:O4'    | 2.25                     | 0.55              |
| 29:DC:51:PRO:CG  | 29:DC:204:ALA:HB2 | 2.35                     | 0.55              |
| 31:DE:151:TYR:O  | 31:DE:153:GLY:N   | 2.40                     | 0.55              |
| 31:DE:2:LYS:CE   | 31:DE:95:ILE:HG23 | 2.35                     | 0.55              |
| 33:DG:20:ILE:HA  | 33:DG:25:TYR:HD2  | 1.70                     | 0.55              |
| 35:DI:5:LEU:N    | 35:DI:5:LEU:HD12  | 2.19                     | 0.55              |
| 38:DP:47:ASP:OD1 | 38:DP:49:ARG:HG3  | 2.06                     | 0.55              |
| 38:DP:48:PRO:CG  | 38:DP:49:ARG:N    | 2.62                     | 0.55              |
| 41:DS:12:PHE:O   | 41:DS:12:PHE:HD1  | 1.89                     | 0.55              |
| 42:DT:86:ILE:O   | 42:DT:86:ILE:HG23 | 2.06                     | 0.55              |
| 1:AA:1072:G:O2'  | 1:AA:1073:U:H5'   | 2.06                     | 0.55              |
| 1:AA:10:A:O2'    | 1:AA:11:G:H5'     | 2.07                     | 0.55              |
| 1:AA:1142:G:C8   | 1:AA:1143:G:C8    | 2.94                     | 0.55              |
| 1:AA:1404:C:H2'  | 1:AA:1405:G:H8    | 1.72                     | 0.55              |
| 1:AA:1459:C:H2'  | 1:AA:1460:A:O4'   | 2.07                     | 0.55              |
| 1:AA:1483:A:H2'  | 1:AA:1484:C:O4'   | 2.07                     | 0.55              |
| 1:AA:278:G:OP2   | 17:AQ:41:LYS:HE2  | 2.07                     | 0.55              |
| 1:AA:315:A:O2'   | 1:AA:316:G:OP2    | 2.21                     | 0.55              |
| 1:AA:538:G:O2'   | 1:AA:539:A:H5'    | 2.07                     | 0.55              |
| 1:AA:662:G:O2'   | 1:AA:663:A:H5'    | 2.06                     | 0.55              |
| 1:AA:675:A:O2'   | 1:AA:676:A:H5'    | 2.07                     | 0.55              |
| 1:AA:962:C:H2'   | 1:AA:963:G:O4'    | 2.07                     | 0.55              |
| 4:AD:98:GLU:C    | 4:AD:100:ARG:N    | 2.57                     | 0.55              |
| 4:AD:31:CYS:O    | 4:AD:31:CYS:SG    | 2.64                     | 0.55              |
| 4:AD:58:LEU:C    | 4:AD:58:LEU:HD13  | 2.27                     | 0.55              |
| 6:AF:2:ARG:CD    | 6:AF:69:GLU:HB3   | 2.34                     | 0.55              |
| 7:AG:74:GLU:OE1  | 7:AG:91:VAL:HG13  | 2.06                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:45:ALA:O     | 9:AI:47:LEU:N      | 2.35                     | 0.55              |
| 10:AJ:34:VAL:CG2  | 10:AJ:74:ILE:HG22  | 2.36                     | 0.55              |
| 13:AM:72:ALA:O    | 13:AM:75:ALA:HB3   | 2.06                     | 0.55              |
| 17:AQ:68:ARG:O    | 17:AQ:68:ARG:HG3   | 2.06                     | 0.55              |
| 51:B2:9:GLN:HE22  | 51:B2:56:GLN:HG2   | 1.71                     | 0.55              |
| 27:BA:1943:U:O4'  | 27:BA:1945:G:H5'   | 2.07                     | 0.55              |
| 27:BA:2047:U:C2'  | 27:BA:2048:G:C5'   | 2.85                     | 0.55              |
| 27:BA:2082:A:O2'  | 27:BA:2083:G:H5'   | 2.07                     | 0.55              |
| 27:BA:2266:A:N3   | 27:BA:2272:U:C4    | 2.75                     | 0.55              |
| 27:BA:690:G:H2'   | 27:BA:691:C:C6     | 2.42                     | 0.55              |
| 27:BA:725:G:H2'   | 27:BA:726:G:O4'    | 2.06                     | 0.55              |
| 27:BA:958:U:O4    | 39:BQ:40:ALA:HA    | 2.06                     | 0.55              |
| 28:BB:29:A:H2'    | 28:BB:30:C:C6      | 2.42                     | 0.55              |
| 33:BG:137:GLU:HB2 | 33:BG:140:ILE:HD11 | 1.88                     | 0.55              |
| 37:BO:97:ARG:HA   | 37:BO:117:LEU:CD2  | 2.36                     | 0.55              |
| 28:BB:52:A:N7     | 41:BS:33:LYS:HE3   | 2.22                     | 0.55              |
| 42:BT:23:ARG:HG2  | 42:BT:120:ARG:NH1  | 2.22                     | 0.55              |
| 42:BT:28:VAL:O    | 42:BT:29:ARG:HG2   | 2.06                     | 0.55              |
| 43:BU:25:TRP:O    | 43:BU:26:GLY:O     | 2.25                     | 0.55              |
| 44:BV:2:PHE:CZ    | 44:BV:4:ILE:HG13   | 2.42                     | 0.55              |
| 27:BA:494:G:O2'   | 45:BW:5:ALA:O      | 2.24                     | 0.55              |
| 47:BY:97:ARG:HG3  | 47:BY:98:VAL:HG23  | 1.89                     | 0.55              |
| 1:CA:451:A:H1'    | 1:CA:452:A:N7      | 2.22                     | 0.55              |
| 1:CA:584:G:H2'    | 1:CA:585:G:H8      | 1.72                     | 0.55              |
| 1:CA:649:G:H8     | 1:CA:649:G:O5'     | 1.90                     | 0.55              |
| 3:CC:156:ARG:HH21 | 3:CC:161:GLU:CG    | 2.16                     | 0.55              |
| 3:CC:92:ALA:HB2   | 3:CC:99:VAL:HG21   | 1.87                     | 0.55              |
| 4:CD:132:ARG:HH11 | 4:CD:132:ARG:HG2   | 1.71                     | 0.55              |
| 4:CD:14:ARG:HB2   | 4:CD:40:PRO:HD3    | 1.88                     | 0.55              |
| 11:CK:80:VAL:HG23 | 11:CK:80:VAL:O     | 2.07                     | 0.55              |
| 14:CN:27:CYS:O    | 14:CN:29:ARG:N     | 2.39                     | 0.55              |
| 14:CN:8:GLU:OE2   | 14:CN:8:GLU:HA     | 2.07                     | 0.55              |
| 25:CY:58:A:H2'    | 25:CY:59:U:H5'     | 1.89                     | 0.55              |
| 49:D0:50:ASN:C    | 49:D0:62:LEU:HD12  | 2.27                     | 0.55              |
| 50:D1:18:ILE:HG21 | 50:D1:20:ARG:CZ    | 2.36                     | 0.55              |
| 27:DA:1005:C:H1'  | 27:DA:1012:U:H3    | 1.69                     | 0.55              |
| 27:DA:1023:U:H2'  | 27:DA:1024:G:O4'   | 2.06                     | 0.55              |
| 27:DA:1907:G:O2'  | 27:DA:1908:C:H5'   | 2.07                     | 0.55              |
| 27:DA:1972:A:C4   | 27:DA:1973:G:N7    | 2.75                     | 0.55              |
| 27:DA:1999:C:H2'  | 27:DA:2000:G:C8    | 2.42                     | 0.55              |
| 27:DA:239:U:H2'   | 27:DA:240:G:O4'    | 2.07                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:390:A:H1'   | 27:DA:391:G:N7     | 2.22                     | 0.55              |
| 29:DC:41:VAL:CB   | 29:DC:213:TYR:HA   | 2.36                     | 0.55              |
| 30:DD:18:VAL:HG13 | 30:DD:211:ARG:NH2  | 2.13                     | 0.55              |
| 31:DE:39:PRO:CG   | 31:DE:45:THR:OG1   | 2.55                     | 0.55              |
| 32:DF:131:GLY:O   | 32:DF:132:VAL:O    | 2.25                     | 0.55              |
| 33:DG:58:GLN:O    | 33:DG:62:LEU:HD13  | 2.07                     | 0.55              |
| 34:DH:40:GLU:O    | 34:DH:42:ARG:N     | 2.39                     | 0.55              |
| 35:DI:28:ASN:C    | 35:DI:32:PRO:HG2   | 2.27                     | 0.55              |
| 45:DW:74:ALA:O    | 45:DW:75:TYR:HB3   | 2.05                     | 0.55              |
| 48:DZ:170:ILE:O   | 48:DZ:171:ALA:HB2  | 2.05                     | 0.55              |
| 1:AA:359:U:H2'    | 1:AA:360:A:H8      | 1.72                     | 0.55              |
| 2:AB:31:TYR:O     | 2:AB:42:ILE:HG13   | 2.07                     | 0.55              |
| 19:AS:48:THR:HA   | 19:AS:61:TYR:O     | 2.06                     | 0.55              |
| 24:AX:1:C:N4      | 24:AX:73:A:C2      | 2.75                     | 0.55              |
| 52:B3:4:LEU:O     | 52:B3:36:VAL:HA    | 2.07                     | 0.55              |
| 27:BA:1887:C:H2'  | 27:BA:1888:G:C5'   | 2.35                     | 0.55              |
| 27:BA:2344:U:H6   | 27:BA:2344:U:O5'   | 1.88                     | 0.55              |
| 27:BA:2427:C:H5'' | 27:BA:2429:G:H5'   | 1.88                     | 0.55              |
| 27:BA:2482:G:H2'  | 27:BA:2483:C:H6    | 1.70                     | 0.55              |
| 27:BA:2537:U:H2'  | 27:BA:2538:C:C6    | 2.42                     | 0.55              |
| 27:BA:2671:A:C2   | 27:BA:2672:G:C4    | 2.95                     | 0.55              |
| 27:BA:664:C:O2'   | 27:BA:665:C:H5'    | 2.07                     | 0.55              |
| 27:BA:846:C:C2    | 27:BA:930:U:C5     | 2.95                     | 0.55              |
| 27:BA:92:A:C1'    | 27:BA:93:G:H8      | 2.19                     | 0.55              |
| 30:BD:28:GLU:CD   | 30:BD:28:GLU:N     | 2.60                     | 0.55              |
| 27:BA:1565:C:P    | 30:BD:4:LYS:NZ     | 2.80                     | 0.55              |
| 31:BE:9:VAL:HG13  | 31:BE:25:VAL:HB    | 1.87                     | 0.55              |
| 34:BH:92:ILE:CG2  | 34:BH:93:GLY:H     | 2.11                     | 0.55              |
| 36:BN:62:VAL:HG21 | 36:BN:67:LEU:HG    | 1.89                     | 0.55              |
| 38:BP:65:ARG:O    | 38:BP:68:GLN:OE1   | 2.24                     | 0.55              |
| 39:BQ:26:TYR:CE1  | 39:BQ:28:ALA:HB2   | 2.42                     | 0.55              |
| 41:BS:24:LEU:CB   | 41:BS:85:VAL:HG12  | 2.28                     | 0.55              |
| 45:BW:79:GLY:O    | 45:BW:100:THR:HG22 | 2.06                     | 0.55              |
| 1:CA:406:G:H5''   | 4:CD:5:ILE:HG21    | 1.89                     | 0.55              |
| 1:CA:532:A:N6     | 3:CC:156:ARG:HH12  | 2.04                     | 0.55              |
| 1:CA:853:G:H2'    | 1:CA:854:G:H8      | 1.72                     | 0.55              |
| 2:CB:22:LYS:O     | 2:CB:24:TRP:CD1    | 2.60                     | 0.55              |
| 6:CF:75:LEU:CD2   | 6:CF:79:LEU:HD11   | 2.37                     | 0.55              |
| 9:CI:63:ILE:CG2   | 9:CI:64:THR:N      | 2.69                     | 0.55              |
| 12:CL:38:ARG:CZ   | 12:CL:38:ARG:HB3   | 2.36                     | 0.55              |
| 13:CM:8:GLU:OE1   | 13:CM:22:ILE:HG12  | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:CO:37:ASN:O     | 15:CO:38:ARG:C     | 2.44                     | 0.55              |
| 20:CT:50:GLU:CB    | 20:CT:100:ILE:HG12 | 2.37                     | 0.55              |
| 55:D6:11:LEU:CD1   | 55:D6:12:GLU:H     | 2.17                     | 0.55              |
| 57:D8:28:GLY:O     | 57:D8:32:LEU:HG    | 2.07                     | 0.55              |
| 27:DA:1022:G:O2'   | 27:DA:1023:U:P     | 2.64                     | 0.55              |
| 27:DA:1426:G:O5'   | 27:DA:1426:G:H8    | 1.90                     | 0.55              |
| 27:DA:2146:C:H5'   | 27:DA:2147:G:N3    | 2.21                     | 0.55              |
| 27:DA:2302:G:N2    | 33:DG:128:ARG:HD2  | 2.21                     | 0.55              |
| 27:DA:2360:A:H2'   | 27:DA:2361:A:O4'   | 2.07                     | 0.55              |
| 27:DA:2697:G:H2'   | 27:DA:2698:U:O4'   | 2.07                     | 0.55              |
| 27:DA:391:G:O2'    | 27:DA:392:C:H5'    | 2.07                     | 0.55              |
| 27:DA:2680:C:H4'   | 31:DE:188:VAL:O    | 2.07                     | 0.55              |
| 31:DE:69:LYS:C     | 31:DE:71:GLY:H     | 2.09                     | 0.55              |
| 32:DF:4:VAL:HG12   | 32:DF:17:ARG:HD3   | 1.88                     | 0.55              |
| 34:DH:147:ASN:N    | 34:DH:147:ASN:ND2  | 2.52                     | 0.55              |
| 37:DO:16:ALA:HB2   | 37:DO:52:VAL:HG13  | 1.88                     | 0.55              |
| 38:DP:45:LEU:CD2   | 38:DP:46:LYS:N     | 2.55                     | 0.55              |
| 39:DQ:109:VAL:HG22 | 39:DQ:113:GLN:OE1  | 2.07                     | 0.55              |
| 40:DR:23:ASN:N     | 40:DR:23:ASN:ND2   | 2.55                     | 0.55              |
| 42:DT:92:GLY:N     | 42:DT:116:ALA:HA   | 2.22                     | 0.55              |
| 48:DZ:164:VAL:HG12 | 48:DZ:165:SER:N    | 2.21                     | 0.55              |
| 48:DZ:94:PRO:HA    | 48:DZ:127:VAL:O    | 2.07                     | 0.55              |
| 1:AA:1305:G:O2'    | 1:AA:1306:A:P      | 2.65                     | 0.55              |
| 1:AA:1361:G:H2'    | 1:AA:1362:C:O4'    | 2.06                     | 0.55              |
| 1:AA:417:C:H2'     | 1:AA:418:C:H6      | 1.72                     | 0.55              |
| 1:AA:539:A:H2'     | 1:AA:540:G:C8      | 2.42                     | 0.55              |
| 1:AA:62:U:O2'      | 1:AA:63:C:H5'      | 2.07                     | 0.55              |
| 1:AA:979:C:C2'     | 1:AA:980:C:H5''    | 2.36                     | 0.55              |
| 3:AC:34:LEU:HD23   | 3:AC:35:GLU:N      | 2.22                     | 0.55              |
| 5:AE:20:GLN:OE1    | 5:AE:25:ARG:NH1    | 2.40                     | 0.55              |
| 12:AL:99:ARG:O     | 12:AL:101:VAL:HG23 | 2.06                     | 0.55              |
| 15:AO:39:LEU:O     | 15:AO:41:GLU:N     | 2.40                     | 0.55              |
| 25:AY:37:U:H3'     | 25:AY:38:U:H5''    | 1.89                     | 0.55              |
| 55:B6:51:GLU:O     | 55:B6:52:VAL:HG23  | 2.07                     | 0.55              |
| 27:BA:1022:G:N2    | 27:BA:1142(A):A:C2 | 2.75                     | 0.55              |
| 27:BA:1175:U:H6    | 27:BA:1178:C:N4    | 2.05                     | 0.55              |
| 27:BA:1821:A:H2'   | 27:BA:1822:G:H8    | 1.72                     | 0.55              |
| 27:BA:2097:C:H2'   | 27:BA:2098:U:H6    | 1.72                     | 0.55              |
| 27:BA:2307:G:OP1   | 27:BA:2307:G:H4'   | 2.07                     | 0.55              |
| 27:BA:2415:G:C4'   | 38:BP:66:GLY:HA3   | 2.37                     | 0.55              |
| 27:BA:271(Y):U:O2' | 27:BA:271(Z):C:O5' | 2.25                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:962:G:O2'    | 27:BA:963:U:H5'   | 2.07                     | 0.55              |
| 29:BC:38:ASP:O     | 29:BC:180:PHE:HA  | 2.07                     | 0.55              |
| 31:BE:36:ARG:HG2   | 31:BE:36:ARG:HH11 | 1.72                     | 0.55              |
| 32:BF:18:ARG:HG3   | 32:BF:19:GLU:N    | 2.22                     | 0.55              |
| 33:BG:13:GLU:O     | 33:BG:14:GLU:HB2  | 2.06                     | 0.55              |
| 38:BP:25:SER:O     | 38:BP:30:THR:HG23 | 2.06                     | 0.55              |
| 41:BS:88:ASP:O     | 41:BS:92:TYR:HB3  | 2.06                     | 0.55              |
| 42:BT:55:ASN:O     | 42:BT:57:PHE:O    | 2.24                     | 0.55              |
| 44:BV:31:ALA:O     | 44:BV:61:VAL:HG12 | 2.06                     | 0.55              |
| 1:CA:1254:C:H41    | 10:CJ:43:ARG:HH12 | 1.55                     | 0.55              |
| 1:CA:174:C:H2'     | 1:CA:175:C:C6     | 2.42                     | 0.55              |
| 1:CA:652:U:O2'     | 1:CA:653:A:N3     | 2.32                     | 0.55              |
| 9:CI:21:PRO:HA     | 9:CI:58:HIS:O     | 2.06                     | 0.55              |
| 11:CK:46:GLY:HA2   | 11:CK:50:TYR:O    | 2.07                     | 0.55              |
| 13:CM:65:LYS:NZ    | 13:CM:65:LYS:CB   | 2.70                     | 0.55              |
| 54:D5:31:VAL:HG23  | 54:D5:40:LYS:HE2  | 1.89                     | 0.55              |
| 55:D6:17:LYS:O     | 55:D6:18:ARG:HD3  | 2.07                     | 0.55              |
| 55:D6:11:LEU:HD11  | 55:D6:52:VAL:C    | 2.27                     | 0.55              |
| 27:DA:1563:G:O2'   | 27:DA:1564:C:H5'  | 2.07                     | 0.55              |
| 27:DA:1722:A:N1    | 27:DA:1740:G:C8   | 2.73                     | 0.55              |
| 27:DA:2069:G:N2    | 27:DA:2070:G:C4   | 2.74                     | 0.55              |
| 27:DA:2275:C:O2'   | 27:DA:2276:G:P    | 2.64                     | 0.55              |
| 27:DA:499:U:H2'    | 27:DA:500:G:H5'   | 1.89                     | 0.55              |
| 27:DA:644:A:H2'    | 27:DA:646:A:C2    | 2.42                     | 0.55              |
| 27:DA:923:C:H2'    | 27:DA:924:C:C6    | 2.42                     | 0.55              |
| 27:DA:962:G:C2'    | 27:DA:963:U:H5'   | 2.37                     | 0.55              |
| 32:DF:170:LEU:HD23 | 32:DF:173:VAL:CG2 | 2.35                     | 0.55              |
| 34:DH:150:ALA:O    | 34:DH:152:ARG:N   | 2.40                     | 0.55              |
| 38:DP:38:GLN:CG    | 38:DP:39:LYS:H    | 2.09                     | 0.55              |
| 40:DR:8:ARG:O      | 40:DR:9:LYS:O     | 2.25                     | 0.55              |
| 44:DV:61:VAL:CA    | 44:DV:94:LEU:HD23 | 2.36                     | 0.55              |
| 1:AA:1002:G:N3     | 1:AA:1002:G:H2'   | 2.21                     | 0.55              |
| 1:AA:1026:G:H3'    | 1:AA:1027:C:H5'   | 1.89                     | 0.55              |
| 1:AA:1189:C:OP1    | 10:AJ:51:ARG:NH2  | 2.34                     | 0.55              |
| 1:AA:745:C:H2'     | 1:AA:746:A:C8     | 2.42                     | 0.55              |
| 3:AC:130:VAL:HG21  | 3:AC:157:ILE:HG23 | 1.89                     | 0.55              |
| 5:AE:78:HIS:CD2    | 8:AH:104:ARG:CZ   | 2.89                     | 0.55              |
| 7:AG:15:ASP:H      | 7:AG:20:ASP:H     | 1.54                     | 0.55              |
| 7:AG:16:LEU:CD1    | 9:AI:42:ARG:HA    | 2.37                     | 0.55              |
| 13:AM:110:ARG:NH1  | 13:AM:110:ARG:HG2 | 2.18                     | 0.55              |
| 15:AO:74:ASP:O     | 15:AO:76:GLU:N    | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:AQ:20:THR:HA   | 17:AQ:42:TYR:O    | 2.07                     | 0.55              |
| 1:AA:128:G:C5'    | 17:AQ:2:PRO:HA    | 2.37                     | 0.55              |
| 17:AQ:59:ILE:HG22 | 17:AQ:71:PHE:HB3  | 1.89                     | 0.55              |
| 20:AT:46:GLU:OE1  | 20:AT:48:LYS:HE2  | 2.07                     | 0.55              |
| 27:BA:1389:G:H2'  | 27:BA:1390:U:C6   | 2.42                     | 0.55              |
| 27:BA:1783:A:C2   | 27:BA:2588:G:O4'  | 2.60                     | 0.55              |
| 27:BA:2220:G:H2'  | 27:BA:2221:G:H8   | 1.71                     | 0.55              |
| 27:BA:2313:C:N4   | 27:BA:2314:C:N4   | 2.55                     | 0.55              |
| 27:BA:2552:U:H2'  | 27:BA:2554:U:H5'' | 1.89                     | 0.55              |
| 27:BA:2650:U:O2'  | 27:BA:2651:C:H5'  | 2.07                     | 0.55              |
| 27:BA:2873:A:H4'  | 27:BA:2874:C:OP1  | 2.07                     | 0.55              |
| 29:BC:121:GLY:HA2 | 29:BC:145:VAL:HA  | 1.89                     | 0.55              |
| 30:BD:77:ALA:HB1  | 30:BD:96:HIS:O    | 2.07                     | 0.55              |
| 43:BU:92:ARG:NH2  | 44:BV:11:GLN:N    | 2.55                     | 0.55              |
| 44:BV:15:GLU:HB3  | 44:BV:16:PRO:CD   | 2.35                     | 0.55              |
| 1:CA:1160:G:O2'   | 1:CA:1161:C:C5'   | 2.55                     | 0.55              |
| 1:CA:565:U:H2'    | 1:CA:566:G:C8     | 2.42                     | 0.55              |
| 1:CA:990:C:H2'    | 1:CA:991:U:H6     | 1.72                     | 0.55              |
| 2:CB:112:VAL:HA   | 2:CB:115:LEU:HB3  | 1.89                     | 0.55              |
| 3:CC:72:LYS:O     | 3:CC:75:VAL:HG23  | 2.07                     | 0.55              |
| 4:CD:101:LEU:CD2  | 4:CD:138:TYR:HB3  | 2.37                     | 0.55              |
| 5:CE:107:ARG:HG2  | 5:CE:108:ALA:N    | 2.21                     | 0.55              |
| 5:CE:45:PHE:CE1   | 5:CE:47:LYS:HG3   | 2.42                     | 0.55              |
| 9:CI:55:ALA:HB1   | 9:CI:59:PHE:CE1   | 2.42                     | 0.55              |
| 10:CJ:96:ILE:O    | 10:CJ:97:GLU:HG2  | 2.06                     | 0.55              |
| 11:CK:127:LYS:CE  | 11:CK:127:LYS:HA  | 2.33                     | 0.55              |
| 12:CL:121:LYS:HG3 | 12:CL:122:PRO:HD2 | 1.88                     | 0.55              |
| 15:CO:83:GLU:O    | 15:CO:86:GLY:N    | 2.38                     | 0.55              |
| 18:CR:44:LEU:HD23 | 18:CR:50:ILE:HA   | 1.88                     | 0.55              |
| 19:CS:66:MET:SD   | 19:CS:74:PHE:HE1  | 2.30                     | 0.55              |
| 23:CW:59:U:H5'    | 23:CW:60:C:OP2    | 2.06                     | 0.55              |
| 24:CX:59:A:C2'    | 24:CX:60:U:H5'    | 2.37                     | 0.55              |
| 52:D3:23:LEU:N    | 52:D3:23:LEU:CD1  | 2.68                     | 0.55              |
| 53:D4:36:VAL:HG13 | 53:D4:52:SER:O    | 2.07                     | 0.55              |
| 27:DA:1565:C:O2'  | 27:DA:1566:A:O5'  | 2.23                     | 0.55              |
| 27:DA:1700:A:H2'  | 27:DA:1701:A:C8   | 2.41                     | 0.55              |
| 27:DA:2301:C:H6   | 27:DA:2301:C:H3'  | 1.70                     | 0.55              |
| 27:DA:2385:C:O2'  | 27:DA:2386:C:H5'  | 2.06                     | 0.55              |
| 27:DA:2700:C:O2'  | 27:DA:2701:C:H5'  | 2.07                     | 0.55              |
| 27:DA:2827:C:O2   | 27:DA:2827:C:H2'  | 2.06                     | 0.55              |
| 27:DA:852:G:H2'   | 27:DA:853:G:C8    | 2.40                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DE:173:VAL:O    | 31:DE:173:VAL:HG12 | 2.06                     | 0.55              |
| 32:DF:128:ALA:O    | 32:DF:129:PHE:C    | 2.45                     | 0.55              |
| 34:DH:89:ILE:HD12  | 34:DH:90:LYS:O     | 2.07                     | 0.55              |
| 36:DN:112:LEU:HD11 | 36:DN:116:LEU:HG   | 1.89                     | 0.55              |
| 38:DP:110:TYR:O    | 38:DP:111:ARG:C    | 2.46                     | 0.55              |
| 41:DS:12:PHE:O     | 41:DS:12:PHE:CD1   | 2.60                     | 0.55              |
| 41:DS:18:ILE:HG22  | 41:DS:18:ILE:O     | 2.07                     | 0.55              |
| 44:DV:40:LEU:N     | 44:DV:40:LEU:CD2   | 2.70                     | 0.55              |
| 46:DX:3:THR:HA     | 46:DX:6:ASP:OD2    | 2.07                     | 0.55              |
| 47:DY:45:VAL:HA    | 47:DY:62:GLU:CG    | 2.37                     | 0.55              |
| 48:DZ:68:THR:HA    | 48:DZ:88:PHE:O     | 2.07                     | 0.55              |
| 1:AA:1134:G:N2     | 1:AA:1141:C:C2     | 2.74                     | 0.54              |
| 1:AA:386:C:O2'     | 1:AA:387:U:H5'     | 2.06                     | 0.54              |
| 1:AA:397:A:N7      | 1:AA:547:A:O2'     | 2.40                     | 0.54              |
| 1:AA:641:U:H5''    | 1:AA:642:A:OP1     | 2.06                     | 0.54              |
| 1:AA:975:A:C4'     | 1:AA:976:G:H5''    | 2.31                     | 0.54              |
| 2:AB:197:VAL:O     | 2:AB:200:ILE:HG13  | 2.07                     | 0.54              |
| 2:AB:51:LEU:O      | 2:AB:55:PHE:HD2    | 1.90                     | 0.54              |
| 5:AE:132:ALA:O     | 5:AE:134:ALA:N     | 2.40                     | 0.54              |
| 5:AE:71:LEU:HD13   | 5:AE:114:GLY:O     | 2.07                     | 0.54              |
| 7:AG:73:MET:HG2    | 7:AG:89:MET:O      | 2.07                     | 0.54              |
| 8:AH:84:ARG:HG2    | 8:AH:84:ARG:NH1    | 2.13                     | 0.54              |
| 11:AK:99:GLN:NE2   | 11:AK:105:VAL:HG21 | 2.22                     | 0.54              |
| 11:AK:21:ILE:HG13  | 11:AK:30:VAL:HB    | 1.88                     | 0.54              |
| 11:AK:48:ILE:HG22  | 11:AK:49:GLY:N     | 2.21                     | 0.54              |
| 12:AL:42:PRO:CB    | 12:AL:89:ASP:HB3   | 2.37                     | 0.54              |
| 1:AA:1204:A:P      | 14:AN:3:ARG:HH12   | 2.30                     | 0.54              |
| 14:AN:40:CYS:SG    | 14:AN:43:CYS:SG    | 3.02                     | 0.54              |
| 17:AQ:76:LEU:HD12  | 17:AQ:77:VAL:H     | 1.72                     | 0.54              |
| 25:AY:72:G:H2'     | 25:AY:73:C:C6      | 2.42                     | 0.54              |
| 51:B2:53:LEU:C     | 51:B2:57:ILE:HG12  | 2.27                     | 0.54              |
| 58:B9:26:ILE:N     | 58:B9:26:ILE:CD1   | 2.70                     | 0.54              |
| 27:BA:1048:A:C2    | 27:BA:1048:A:OP2   | 2.60                     | 0.54              |
| 27:BA:1109:C:H5''  | 27:BA:1110:G:OP2   | 2.07                     | 0.54              |
| 27:BA:11:G:C2'     | 27:BA:12:U:H5'     | 2.37                     | 0.54              |
| 27:BA:1361:G:O2'   | 27:BA:1362:C:H5'   | 2.07                     | 0.54              |
| 27:BA:2145:C:H3'   | 27:BA:2145:C:H6    | 1.71                     | 0.54              |
| 27:BA:2163:C:H2'   | 27:BA:2164:C:H5'   | 1.88                     | 0.54              |
| 27:BA:2682:U:O4'   | 31:BE:12:THR:HA    | 2.07                     | 0.54              |
| 27:BA:722:A:N3     | 27:BA:722:A:H2'    | 2.22                     | 0.54              |
| 27:BA:80:G:C6      | 27:BA:81:G:C5      | 2.96                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:860:U:H2'    | 27:BA:861:A:H8     | 1.72                     | 0.54              |
| 27:BA:908:C:O2'    | 27:BA:909:A:H5'    | 2.07                     | 0.54              |
| 27:BA:937:U:H2'    | 27:BA:938:G:H8     | 1.71                     | 0.54              |
| 30:BD:28:GLU:H     | 30:BD:29:PRO:HD2   | 1.72                     | 0.54              |
| 32:BF:11:VAL:HG12  | 32:BF:12:LEU:N     | 2.12                     | 0.54              |
| 34:BH:118:PRO:HG2  | 34:BH:121:ILE:HB   | 1.88                     | 0.54              |
| 35:BI:73:GLU:HA    | 35:BI:138:ILE:HG23 | 1.88                     | 0.54              |
| 37:BO:36:GLY:HA3   | 37:BO:109:LYS:HG3  | 1.90                     | 0.54              |
| 39:BQ:137:TYR:N    | 39:BQ:137:TYR:HD2  | 2.05                     | 0.54              |
| 40:BR:17:ARG:HH11  | 40:BR:17:ARG:HG2   | 1.72                     | 0.54              |
| 45:BW:68:ARG:NH1   | 45:BW:111:HIS:CD2  | 2.75                     | 0.54              |
| 39:BQ:134:ARG:NH2  | 48:BZ:118:GLU:OE1  | 2.36                     | 0.54              |
| 48:BZ:144:GLU:O    | 48:BZ:146:GLY:N    | 2.39                     | 0.54              |
| 1:CA:176:C:H2'     | 1:CA:177:C:H6      | 1.72                     | 0.54              |
| 1:CA:189(L):G:H2'  | 1:CA:190:U:H6      | 1.64                     | 0.54              |
| 1:CA:222:U:H2'     | 1:CA:223:U:H6      | 1.71                     | 0.54              |
| 1:CA:31:G:N7       | 1:CA:306:G:H1'     | 2.22                     | 0.54              |
| 7:CG:123:GLU:OE2   | 7:CG:123:GLU:HA    | 2.07                     | 0.54              |
| 1:CA:1151:A:H5''   | 10:CJ:42:THR:H     | 1.72                     | 0.54              |
| 10:CJ:74:ILE:O     | 10:CJ:74:ILE:HG13  | 2.07                     | 0.54              |
| 12:CL:107:VAL:HG12 | 12:CL:110:ARG:HB2  | 1.89                     | 0.54              |
| 12:CL:34:CYS:SG    | 12:CL:78:SER:HB2   | 2.48                     | 0.54              |
| 11:CK:111:ASP:CA   | 18:CR:84:LYS:HG3   | 2.35                     | 0.54              |
| 19:CS:33:THR:O     | 19:CS:57:HIS:CE1   | 2.59                     | 0.54              |
| 23:CW:70:C:O2'     | 23:CW:71:A:O5'     | 2.25                     | 0.54              |
| 27:DA:2267:A:H3'   | 27:DA:2268:A:C5'   | 2.36                     | 0.54              |
| 27:DA:2316:C:H2'   | 27:DA:2316:C:O2    | 2.06                     | 0.54              |
| 27:DA:2729:G:H1'   | 31:DE:187:ALA:HB3  | 1.89                     | 0.54              |
| 27:DA:272(G):C:H42 | 27:DA:363(C):G:H1  | 1.54                     | 0.54              |
| 27:DA:2856:C:O2    | 27:DA:2856:C:H2'   | 2.05                     | 0.54              |
| 27:DA:301:G:H1'    | 27:DA:302:C:C6     | 2.42                     | 0.54              |
| 27:DA:325:G:H2'    | 27:DA:326:G:C8     | 2.42                     | 0.54              |
| 27:DA:346:A:O2'    | 27:DA:347:A:H5'    | 2.07                     | 0.54              |
| 28:DB:52:A:N7      | 41:DS:33:LYS:HE3   | 2.22                     | 0.54              |
| 29:DC:47:LEU:HB3   | 29:DC:207:THR:HA   | 1.89                     | 0.54              |
| 30:DD:210:GLY:O    | 30:DD:211:ARG:HB3  | 2.07                     | 0.54              |
| 32:DF:61:GLY:O     | 32:DF:62:ARG:O     | 2.26                     | 0.54              |
| 34:DH:113:VAL:HG12 | 34:DH:115:VAL:HG22 | 1.89                     | 0.54              |
| 37:DO:115:VAL:O    | 37:DO:118:ALA:HB3  | 2.06                     | 0.54              |
| 40:DR:89:ASP:O     | 40:DR:90:ARG:HB2   | 2.07                     | 0.54              |
| 46:DX:50:LYS:O     | 46:DX:83:VAL:HG12  | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:DY:15:VAL:HG12  | 47:DY:16:ALA:N     | 2.22                     | 0.54              |
| 47:DY:45:VAL:HA    | 47:DY:62:GLU:OE2   | 2.07                     | 0.54              |
| 1:AA:383:A:H2'     | 1:AA:384:G:H5'     | 1.89                     | 0.54              |
| 1:AA:999:C:H42     | 1:AA:1042:G:H22    | 1.55                     | 0.54              |
| 2:AB:87:ARG:HD2    | 2:AB:87:ARG:O      | 2.07                     | 0.54              |
| 5:AE:20:GLN:NE2    | 5:AE:25:ARG:CZ     | 2.66                     | 0.54              |
| 6:AF:12:PRO:O      | 6:AF:14:LEU:N      | 2.33                     | 0.54              |
| 8:AH:53:VAL:O      | 8:AH:56:LYS:N      | 2.25                     | 0.54              |
| 11:AK:57:THR:HG22  | 11:AK:58:PRO:HD2   | 1.89                     | 0.54              |
| 7:AG:153:HIS:CB    | 11:AK:58:PRO:HG3   | 2.37                     | 0.54              |
| 12:AL:123:LYS:HD2  | 12:AL:124:GLU:H    | 1.71                     | 0.54              |
| 13:AM:75:ALA:C     | 13:AM:79:LYS:HZ2   | 2.09                     | 0.54              |
| 15:AO:33:THR:HG23  | 15:AO:63:ARG:NH1   | 2.20                     | 0.54              |
| 16:AP:15:PRO:C     | 16:AP:16:HIS:ND1   | 2.60                     | 0.54              |
| 20:AT:12:ALA:C     | 20:AT:14:LYS:H     | 2.09                     | 0.54              |
| 20:AT:43:LEU:HB3   | 20:AT:48:LYS:HG3   | 1.90                     | 0.54              |
| 51:B2:32:LEU:CB    | 51:B2:53:LEU:HD12  | 2.37                     | 0.54              |
| 27:BA:1289:C:H5'   | 27:BA:1289:C:C6    | 2.36                     | 0.54              |
| 27:BA:1494:A:N3    | 27:BA:1494:A:C2'   | 2.70                     | 0.54              |
| 27:BA:1556:C:H2'   | 27:BA:1557:C:C6    | 2.42                     | 0.54              |
| 27:BA:1676:A:O5'   | 27:BA:1676:A:H8    | 1.90                     | 0.54              |
| 27:BA:2110:G:OP2   | 27:BA:2110:G:H8    | 1.91                     | 0.54              |
| 27:BA:2580:U:H5''  | 31:BE:131:ALA:HB2  | 1.89                     | 0.54              |
| 27:BA:2680:C:H5'   | 31:BE:189:PRO:CA   | 2.19                     | 0.54              |
| 27:BA:406:G:C8     | 27:BA:406:G:O5'    | 2.57                     | 0.54              |
| 27:BA:633:A:H2'    | 27:BA:634:C:C5'    | 2.37                     | 0.54              |
| 27:BA:686:G:H1'    | 56:B7:6:GLN:O      | 2.07                     | 0.54              |
| 27:BA:684:G:C2     | 27:BA:794:G:C2     | 2.95                     | 0.54              |
| 32:BF:53:THR:H     | 32:BF:56:GLU:HB2   | 1.72                     | 0.54              |
| 34:BH:85:LYS:HE2   | 34:BH:145:ALA:CB   | 2.35                     | 0.54              |
| 35:BI:123:LEU:HD11 | 35:BI:144:VAL:HG12 | 1.90                     | 0.54              |
| 37:BO:10:VAL:HG11  | 37:BO:16:ALA:O     | 2.07                     | 0.54              |
| 41:BS:14:VAL:HG12  | 41:BS:15:ARG:H     | 1.72                     | 0.54              |
| 46:BX:12:VAL:HB    | 46:BX:17:ALA:HB1   | 1.87                     | 0.54              |
| 47:BY:95:LYS:HZ2   | 47:BY:99:CYS:C     | 2.09                     | 0.54              |
| 1:CA:1191:A:H5''   | 3:CC:4:LYS:HZ1     | 1.70                     | 0.54              |
| 1:CA:1305:G:C2     | 1:CA:1331:G:N3     | 2.75                     | 0.54              |
| 1:CA:142:G:H2'     | 1:CA:143:A:H8      | 1.67                     | 0.54              |
| 1:CA:1417:G:H2'    | 1:CA:1482:G:N2     | 2.22                     | 0.54              |
| 1:CA:309:G:C1'     | 1:CA:608:A:H2      | 2.11                     | 0.54              |
| 1:CA:770:C:H2'     | 1:CA:771:G:C8      | 2.42                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:CF:21:LEU:HD13  | 6:CF:24:GLU:OE1   | 2.07                     | 0.54              |
| 10:CJ:24:VAL:HG21 | 10:CJ:37:PRO:HG3  | 1.89                     | 0.54              |
| 13:CM:90:LEU:O    | 13:CM:91:ARG:HB2  | 2.07                     | 0.54              |
| 10:CJ:49:VAL:CG2  | 14:CN:41:ARG:HB2  | 2.37                     | 0.54              |
| 17:CQ:97:SER:O    | 17:CQ:99:SER:N    | 2.38                     | 0.54              |
| 23:CW:70:C:O2'    | 23:CW:71:A:H8     | 1.91                     | 0.54              |
| 26:CZ:3:SER:O     | 26:CZ:4:SER:HB3   | 2.07                     | 0.54              |
| 52:D3:47:VAL:HA   | 52:D3:50:VAL:HG22 | 1.90                     | 0.54              |
| 27:DA:1680:U:H3'  | 27:DA:1681:G:C8   | 2.42                     | 0.54              |
| 27:DA:2014:A:H2'  | 27:DA:2015:A:C8   | 2.43                     | 0.54              |
| 27:DA:2147:G:H2'  | 27:DA:2148:G:C8   | 2.42                     | 0.54              |
| 27:DA:221:A:C4'   | 27:DA:222:A:O5'   | 2.53                     | 0.54              |
| 27:DA:2460:U:C2'  | 27:DA:2461:C:H5'  | 2.37                     | 0.54              |
| 27:DA:2833:G:C3'  | 27:DA:2834:G:C5'  | 2.76                     | 0.54              |
| 27:DA:289:A:N3    | 27:DA:289:A:H2'   | 2.20                     | 0.54              |
| 27:DA:67:U:H2'    | 27:DA:68:G:C8     | 2.37                     | 0.54              |
| 27:DA:813:U:H2'   | 27:DA:814:C:C6    | 2.42                     | 0.54              |
| 27:DA:977:G:O2'   | 27:DA:978:G:H5'   | 2.07                     | 0.54              |
| 28:DB:106:G:H2'   | 28:DB:107:G:H8    | 1.70                     | 0.54              |
| 30:DD:238:GLY:O   | 30:DD:239:ARG:O   | 2.25                     | 0.54              |
| 31:DE:95:ILE:HG22 | 31:DE:96:PHE:CD1  | 2.42                     | 0.54              |
| 32:DF:153:SER:OG  | 32:DF:190:GLU:HG3 | 2.07                     | 0.54              |
| 33:DG:3:LEU:O     | 33:DG:4:ASP:HB3   | 2.07                     | 0.54              |
| 38:DP:7:ARG:HA    | 38:DP:7:ARG:NE    | 2.21                     | 0.54              |
| 38:DP:93:GLY:O    | 38:DP:123:LEU:HB2 | 2.07                     | 0.54              |
| 39:DQ:75:THR:HG21 | 39:DQ:87:LYS:HG3  | 1.88                     | 0.54              |
| 45:DW:18:ARG:HG2  | 45:DW:18:ARG:NH1  | 2.22                     | 0.54              |
| 45:DW:26:GLY:HA2  | 45:DW:71:VAL:O    | 2.08                     | 0.54              |
| 48:DZ:55:VAL:HA   | 48:DZ:69:LEU:CD2  | 2.37                     | 0.54              |
| 48:DZ:60:LEU:HG   | 48:DZ:64:GLN:HB2  | 1.89                     | 0.54              |
| 48:DZ:99:VAL:O    | 48:DZ:122:ASP:HA  | 2.07                     | 0.54              |
| 1:AA:1137:C:C4'   | 1:AA:1138:G:C2    | 2.87                     | 0.54              |
| 1:AA:1220:G:O3'   | 19:AS:36:ARG:HD3  | 2.08                     | 0.54              |
| 1:AA:1306:A:H61   | 1:AA:1331:G:H1'   | 1.72                     | 0.54              |
| 1:AA:1366:C:O2'   | 1:AA:1367:C:H5'   | 2.06                     | 0.54              |
| 1:AA:620:C:N1     | 4:AD:135:LEU:HD23 | 2.22                     | 0.54              |
| 7:AG:69:VAL:HG12  | 7:AG:100:ALA:HA   | 1.89                     | 0.54              |
| 17:AQ:29:HIS:CE1  | 17:AQ:31:LEU:HB3  | 2.38                     | 0.54              |
| 23:AW:27:C:C4     | 23:AW:28:G:N7     | 2.75                     | 0.54              |
| 50:B1:23:LYS:HD3  | 50:B1:28:GLY:HA3  | 1.89                     | 0.54              |
| 55:B6:20:ASN:ND2  | 55:B6:21:TYR:N    | 2.51                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1205:U:H4'   | 27:BA:1206:G:OP2   | 2.07                     | 0.54              |
| 27:BA:1331:A:H3'   | 27:BA:1333:C:H41   | 1.71                     | 0.54              |
| 27:BA:530:G:O6     | 27:BA:2023:G:OP1   | 2.26                     | 0.54              |
| 27:BA:2036:C:O2'   | 27:BA:2037:G:H8    | 1.90                     | 0.54              |
| 27:BA:2048:G:C6    | 27:BA:2621:A:N1    | 2.76                     | 0.54              |
| 27:BA:2164:C:H3'   | 27:BA:2165:G:C8    | 2.42                     | 0.54              |
| 27:BA:2287:A:N1    | 27:BA:2346:A:C2    | 2.75                     | 0.54              |
| 27:BA:576:U:H4'    | 27:BA:2502:G:C8    | 2.42                     | 0.54              |
| 27:BA:2522:U:O2'   | 27:BA:2647:U:OP1   | 2.23                     | 0.54              |
| 27:BA:841:A:H2'    | 27:BA:842:G:C8     | 2.42                     | 0.54              |
| 30:BD:166:GLN:CB   | 30:BD:174:ILE:HG22 | 2.37                     | 0.54              |
| 27:BA:1902:C:H4'   | 30:BD:244:ARG:HA   | 1.89                     | 0.54              |
| 30:BD:24:ILE:O     | 30:BD:26:LYS:HE3   | 2.07                     | 0.54              |
| 32:BF:202:PHE:O    | 32:BF:205:ARG:CB   | 2.54                     | 0.54              |
| 35:BI:140:LEU:HD12 | 35:BI:141:LYS:H    | 1.72                     | 0.54              |
| 36:BN:17:ASP:C     | 36:BN:17:ASP:OD2   | 2.46                     | 0.54              |
| 1:CA:1064:G:H21    | 1:CA:1190:G:H2'    | 1.73                     | 0.54              |
| 1:CA:1165:C:C2'    | 1:CA:1166:G:H5'    | 2.37                     | 0.54              |
| 1:CA:1197:G:O2'    | 1:CA:1198:G:H5'    | 2.07                     | 0.54              |
| 1:CA:1287:A:H2     | 1:CA:1353:G:H1'    | 1.71                     | 0.54              |
| 1:CA:129:U:N3      | 1:CA:131:C:N4      | 2.53                     | 0.54              |
| 1:CA:411:A:C6      | 1:CA:429:U:C5      | 2.95                     | 0.54              |
| 1:CA:606:G:H2'     | 1:CA:631:G:N2      | 2.23                     | 0.54              |
| 1:CA:638:G:H2'     | 1:CA:639:G:C8      | 2.42                     | 0.54              |
| 1:CA:755:G:O2'     | 1:CA:756:C:H5'     | 2.08                     | 0.54              |
| 5:CE:125:SER:OG    | 5:CE:126:ARG:N     | 2.39                     | 0.54              |
| 5:CE:84:PHE:O      | 5:CE:86:ALA:N      | 2.40                     | 0.54              |
| 8:CH:39:LEU:HD21   | 8:CH:111:ILE:HD11  | 1.88                     | 0.54              |
| 9:CI:99:LEU:HD12   | 9:CI:101:PHE:CE1   | 2.42                     | 0.54              |
| 12:CL:5:ASN:HA     | 12:CL:8:VAL:HG21   | 1.90                     | 0.54              |
| 17:CQ:15:MET:HE1   | 17:CQ:43:LEU:HD13  | 1.89                     | 0.54              |
| 50:D1:46:LEU:O     | 50:D1:46:LEU:HD23  | 2.06                     | 0.54              |
| 52:D3:36:VAL:HG23  | 52:D3:36:VAL:O     | 2.07                     | 0.54              |
| 56:D7:10:ARG:O     | 56:D7:13:ALA:HB3   | 2.08                     | 0.54              |
| 57:D8:53:PRO:O     | 57:D8:54:GLU:C     | 2.45                     | 0.54              |
| 27:DA:1170:G:H22   | 27:DA:1179:C:H42   | 1.55                     | 0.54              |
| 27:DA:1195:G:O2'   | 27:DA:1196:C:H5'   | 2.08                     | 0.54              |
| 27:DA:1328:G:O2'   | 27:DA:1329:U:H5''  | 2.07                     | 0.54              |
| 27:DA:1693:U:H2'   | 30:DD:14:ARG:NH2   | 2.22                     | 0.54              |
| 27:DA:1722:A:C6    | 27:DA:1740:G:C8    | 2.95                     | 0.54              |
| 27:DA:1897:G:C2    | 27:DA:1898:U:C2    | 2.95                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2312:U:C2'   | 27:DA:2313:C:H5''  | 2.36                     | 0.54              |
| 27:DA:2445:G:H2'   | 27:DA:2446:G:C8    | 2.42                     | 0.54              |
| 27:DA:2064:C:H1'   | 27:DA:2450:A:N1    | 2.23                     | 0.54              |
| 27:DA:2884:U:C2'   | 27:DA:2885:C:H5'   | 2.37                     | 0.54              |
| 27:DA:391:G:O5'    | 27:DA:391:G:C8     | 2.60                     | 0.54              |
| 27:DA:872:A:N1     | 27:DA:905:U:O2     | 2.40                     | 0.54              |
| 29:DC:24:GLU:HB3   | 29:DC:27:ARG:HH21  | 1.71                     | 0.54              |
| 29:DC:68:LEU:CB    | 29:DC:70:LYS:HE2   | 2.37                     | 0.54              |
| 29:DC:77:ILE:HD11  | 29:DC:100:ILE:HG13 | 1.89                     | 0.54              |
| 30:DD:30:GLU:OE2   | 30:DD:83:GLU:HB3   | 2.07                     | 0.54              |
| 32:DF:127:GLU:HB2  | 32:DF:196:LEU:HD12 | 1.89                     | 0.54              |
| 32:DF:2:LYS:HD3    | 32:DF:2:LYS:H      | 1.70                     | 0.54              |
| 36:DN:67:LEU:HB3   | 36:DN:88:GLU:CG    | 2.37                     | 0.54              |
| 32:DF:188:ARG:N    | 38:DP:7:ARG:HH22   | 2.05                     | 0.54              |
| 41:DS:59:LYS:HE3   | 41:DS:68:GLN:HE22  | 1.72                     | 0.54              |
| 42:DT:105:LEU:HD22 | 42:DT:109:GLU:OE1  | 2.07                     | 0.54              |
| 42:DT:54:ARG:O     | 42:DT:55:ASN:CB    | 2.54                     | 0.54              |
| 1:AA:1161:C:H2'    | 1:AA:1162:C:C6     | 2.43                     | 0.54              |
| 1:AA:402:G:O2'     | 1:AA:403:C:H5'     | 2.08                     | 0.54              |
| 1:AA:484:G:H4'     | 1:AA:485:G:O5'     | 2.07                     | 0.54              |
| 1:AA:944:G:N2      | 1:AA:1338:G:C8     | 2.76                     | 0.54              |
| 1:AA:961:U:OP2     | 1:AA:1223:C:H1'    | 2.07                     | 0.54              |
| 5:AE:43:LEU:CD2    | 5:AE:109:ILE:HD11  | 2.30                     | 0.54              |
| 10:AJ:94:VAL:HG12  | 10:AJ:95:GLU:N     | 2.21                     | 0.54              |
| 18:AR:51:LEU:HD23  | 18:AR:52:PRO:HD2   | 1.89                     | 0.54              |
| 46:BX:13:LEU:HD11  | 51:B2:40:SER:O     | 2.08                     | 0.54              |
| 54:B5:16:ARG:CG    | 54:B5:17:ASP:H     | 2.19                     | 0.54              |
| 55:B6:34:LEU:O     | 55:B6:36:LEU:HD23  | 2.08                     | 0.54              |
| 57:B8:61:LEU:HD12  | 57:B8:61:LEU:N     | 2.23                     | 0.54              |
| 27:BA:1407:C:H5'   | 27:BA:1408:C:OP2   | 2.08                     | 0.54              |
| 27:BA:1674:G:N2    | 27:BA:1677:A:N1    | 2.54                     | 0.54              |
| 27:BA:1790:C:H2'   | 27:BA:1791:A:C4    | 2.43                     | 0.54              |
| 27:BA:1961:C:C2'   | 27:BA:1962:C:H5'   | 2.37                     | 0.54              |
| 27:BA:2028:U:H2'   | 27:BA:2029:G:O4'   | 2.07                     | 0.54              |
| 27:BA:2047:U:C2'   | 27:BA:2048:G:H5'   | 2.37                     | 0.54              |
| 27:BA:2111:C:C5    | 27:BA:2145:C:C4    | 2.95                     | 0.54              |
| 27:BA:2134:A:C2    | 27:BA:2159:G:H1'   | 2.42                     | 0.54              |
| 27:BA:234:C:O2'    | 27:BA:235:U:H5'    | 2.07                     | 0.54              |
| 27:BA:2378:A:N7    | 27:BA:2379:G:H1'   | 2.22                     | 0.54              |
| 27:BA:247:G:H4'    | 27:BA:386:G:C5     | 2.42                     | 0.54              |
| 27:BA:49:A:C8      | 27:BA:51:G:C2      | 2.95                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:836:G:H2'    | 27:BA:837:C:C6     | 2.42                     | 0.54              |
| 27:BA:940:G:H2'    | 27:BA:941:A:C4'    | 2.37                     | 0.54              |
| 28:BB:79:C:H42     | 28:BB:98:G:H1      | 1.54                     | 0.54              |
| 32:BF:110:LEU:C    | 32:BF:110:LEU:HD13 | 2.28                     | 0.54              |
| 32:BF:20:LEU:CD2   | 32:BF:203:GLN:HE22 | 2.20                     | 0.54              |
| 32:BF:2:LYS:HG2    | 32:BF:25:PRO:HG2   | 1.89                     | 0.54              |
| 38:BP:23:PRO:HD2   | 38:BP:33:ARG:HH21  | 1.72                     | 0.54              |
| 42:BT:65:LYS:HA    | 42:BT:65:LYS:NZ    | 2.23                     | 0.54              |
| 43:BU:25:TRP:HD1   | 43:BU:26:GLY:H     | 1.55                     | 0.54              |
| 1:CA:38:G:H4'      | 1:CA:547:A:N6      | 2.21                     | 0.54              |
| 1:CA:981:U:O5'     | 1:CA:981:U:H6      | 1.89                     | 0.54              |
| 2:CB:36:ARG:HA     | 2:CB:36:ARG:CZ     | 2.37                     | 0.54              |
| 6:CF:8:ILE:HD13    | 6:CF:26:ILE:HD13   | 1.89                     | 0.54              |
| 9:CI:83:ARG:NH2    | 9:CI:102:LEU:HD11  | 2.22                     | 0.54              |
| 13:CM:82:MET:O     | 13:CM:82:MET:CG    | 2.54                     | 0.54              |
| 13:CM:95:GLY:O     | 13:CM:96:LEU:HD12  | 2.06                     | 0.54              |
| 17:CQ:12:SER:HA    | 17:CQ:14:LYS:NZ    | 2.22                     | 0.54              |
| 18:CR:47:THR:HA    | 18:CR:83:GLU:O     | 2.08                     | 0.54              |
| 19:CS:29:ARG:O     | 19:CS:31:ILE:HG22  | 2.07                     | 0.54              |
| 20:CT:16:HIS:C     | 20:CT:19:SER:HB3   | 2.28                     | 0.54              |
| 49:D0:34:GLY:O     | 49:D0:35:ASN:C     | 2.45                     | 0.54              |
| 49:D0:53:MET:HB3   | 49:D0:59:LEU:CD2   | 2.31                     | 0.54              |
| 50:D1:20:ARG:O     | 50:D1:21:ARG:HG2   | 2.08                     | 0.54              |
| 27:DA:2019:A:N6    | 27:DA:2035:G:H1    | 2.06                     | 0.54              |
| 27:DA:2543:G:O2'   | 27:DA:2544:G:H5'   | 2.08                     | 0.54              |
| 27:DA:627:A:N3     | 27:DA:636:G:N2     | 2.53                     | 0.54              |
| 27:DA:852:G:C5     | 27:DA:853:G:N7     | 2.75                     | 0.54              |
| 30:DD:211:ARG:HG3  | 30:DD:211:ARG:O    | 2.07                     | 0.54              |
| 30:DD:52:ARG:NH1   | 30:DD:249:PRO:HG2  | 2.23                     | 0.54              |
| 31:DE:11:MET:HE3   | 31:DE:186:GLY:HA2  | 1.89                     | 0.54              |
| 36:DN:41:ASP:O     | 36:DN:42:TRP:C     | 2.46                     | 0.54              |
| 27:DA:2394:C:OP1   | 38:DP:63:PRO:HG2   | 2.07                     | 0.54              |
| 39:DQ:134:ARG:HH21 | 48:DZ:121:ARG:CZ   | 2.21                     | 0.54              |
| 42:DT:3:ARG:C      | 42:DT:5:ALA:N      | 2.59                     | 0.54              |
| 44:DV:43:GLU:O     | 44:DV:44:LYS:HB2   | 2.08                     | 0.54              |
| 46:DX:41:ASN:N     | 46:DX:41:ASN:HD22  | 2.04                     | 0.54              |
| 48:DZ:104:VAL:O    | 48:DZ:104:VAL:HG13 | 2.08                     | 0.54              |
| 1:AA:1149:C:H2'    | 1:AA:1150:U:C6     | 2.42                     | 0.54              |
| 1:AA:537:G:H2'     | 1:AA:538:G:C8      | 2.42                     | 0.54              |
| 1:AA:719:C:C2      | 18:AR:50:ILE:HG12  | 2.42                     | 0.54              |
| 1:AA:841:U:O2'     | 1:AA:848:C:H5'     | 2.07                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:152:SER:C     | 4:AD:154:ASN:H     | 2.10                     | 0.54              |
| 4:AD:152:SER:O     | 4:AD:155:LEU:HG    | 2.08                     | 0.54              |
| 7:AG:54:THR:OG1    | 7:AG:56:GLN:CG     | 2.47                     | 0.54              |
| 1:AA:590:C:OP1     | 8:AH:30:ARG:HB3    | 2.08                     | 0.54              |
| 12:AL:73:ASN:H     | 12:AL:73:ASN:ND2   | 2.04                     | 0.54              |
| 16:AP:22:THR:HG1   | 16:AP:26:ARG:HG3   | 1.70                     | 0.54              |
| 51:B2:13:ALA:O     | 51:B2:15:LYS:N     | 2.39                     | 0.54              |
| 55:B6:39:TYR:HD2   | 55:B6:49:HIS:CD2   | 2.26                     | 0.54              |
| 56:B7:31:LEU:O     | 56:B7:35:ARG:HB2   | 2.08                     | 0.54              |
| 56:B7:45:ALA:O     | 56:B7:46:VAL:CG2   | 2.56                     | 0.54              |
| 57:B8:32:LEU:CB    | 57:B8:36:LYS:HD2   | 2.38                     | 0.54              |
| 27:BA:1200:C:H2'   | 27:BA:1201:C:H6    | 1.73                     | 0.54              |
| 27:BA:1527:G:H5''  | 27:BA:1528:A:OP1   | 2.07                     | 0.54              |
| 27:BA:1804:C:H4'   | 30:BD:252:TRP:CZ2  | 2.43                     | 0.54              |
| 27:BA:1812:A:C2    | 27:BA:1813:G:C5    | 2.95                     | 0.54              |
| 27:BA:2080:G:H2'   | 27:BA:2081:C:H6    | 1.72                     | 0.54              |
| 27:BA:271(U):G:C2' | 27:BA:271(V):G:H5' | 2.37                     | 0.54              |
| 27:BA:216:A:C8     | 27:BA:432:A:C6     | 2.96                     | 0.54              |
| 27:BA:542:C:N4     | 27:BA:543:C:N4     | 2.55                     | 0.54              |
| 33:BG:39:ILE:O     | 33:BG:39:ILE:HG23  | 2.07                     | 0.54              |
| 35:BI:13:GLY:O     | 35:BI:17:GLN:OE1   | 2.25                     | 0.54              |
| 39:BQ:107:ALA:O    | 39:BQ:109:VAL:HG23 | 2.08                     | 0.54              |
| 39:BQ:57:HIS:C     | 39:BQ:57:HIS:CD2   | 2.81                     | 0.54              |
| 27:BA:2851:A:O3'   | 40:BR:64:ARG:NH2   | 2.41                     | 0.54              |
| 42:BT:108:ARG:CA   | 42:BT:111:ARG:HG3  | 2.37                     | 0.54              |
| 47:BY:88:LYS:HB3   | 47:BY:90:LEU:HD12  | 1.89                     | 0.54              |
| 1:CA:61:G:C6       | 1:CA:107:G:N1      | 2.75                     | 0.54              |
| 1:CA:202:U:H5''    | 1:CA:203:U:OP2     | 2.07                     | 0.54              |
| 1:CA:384:G:H2'     | 1:CA:385:C:H6      | 1.70                     | 0.54              |
| 1:CA:599:C:H5''    | 8:CH:96:GLY:HA2    | 1.89                     | 0.54              |
| 3:CC:84:ILE:HA     | 3:CC:87:LEU:HD12   | 1.90                     | 0.54              |
| 11:CK:52:GLY:O     | 11:CK:55:LYS:HG3   | 2.07                     | 0.54              |
| 1:CA:1226:C:OP1    | 19:CS:81:ARG:NH1   | 2.41                     | 0.54              |
| 20:CT:67:ALA:O     | 20:CT:73:HIS:CD2   | 2.61                     | 0.54              |
| 49:D0:27:GLU:N     | 49:D0:69:PHE:HE1   | 2.06                     | 0.54              |
| 55:D6:19:ARG:H     | 55:D6:19:ARG:HD2   | 1.73                     | 0.54              |
| 27:DA:1887:C:C2'   | 27:DA:1888:G:H5''  | 2.37                     | 0.54              |
| 27:DA:2092:U:H4'   | 27:DA:2093:G:O5'   | 2.07                     | 0.54              |
| 27:DA:2430:A:H2'   | 27:DA:2431:U:H5'   | 1.90                     | 0.54              |
| 27:DA:2067:G:H1    | 27:DA:2443:C:N4    | 2.05                     | 0.54              |
| 27:DA:2579:C:O3'   | 31:DE:131:ALA:CB   | 2.45                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2755:C:H3'   | 58:D9:19:ARG:NH2   | 2.23                     | 0.54              |
| 27:DA:526:A:N6     | 27:DA:2626:C:H4'   | 2.23                     | 0.54              |
| 27:DA:950:G:O6     | 27:DA:967:C:N4     | 2.40                     | 0.54              |
| 28:DB:45:A:H1'     | 33:DG:95:ARG:NH1   | 2.22                     | 0.54              |
| 30:DD:173:VAL:CG2  | 30:DD:174:ILE:N    | 2.70                     | 0.54              |
| 31:DE:11:MET:CB    | 31:DE:24:THR:HA    | 2.38                     | 0.54              |
| 33:DG:33:ARG:O     | 33:DG:35:GLU:N     | 2.40                     | 0.54              |
| 38:DP:13:ASN:ND2   | 38:DP:14:LYS:N     | 2.55                     | 0.54              |
| 39:DQ:3:MET:O      | 39:DQ:5:ARG:N      | 2.41                     | 0.54              |
| 40:DR:20:LEU:HG    | 40:DR:21:TYR:CD2   | 2.42                     | 0.54              |
| 42:DT:13:ARG:CA    | 42:DT:13:ARG:NE    | 2.70                     | 0.54              |
| 27:DA:2867:G:C5    | 42:DT:23:ARG:NH1   | 2.75                     | 0.54              |
| 42:DT:82:LEU:O     | 42:DT:83:ILE:C     | 2.45                     | 0.54              |
| 42:DT:96:ARG:CG    | 42:DT:96:ARG:HH11  | 2.09                     | 0.54              |
| 45:DW:11:ARG:N     | 45:DW:100:THR:OG1  | 2.39                     | 0.54              |
| 45:DW:29:LEU:HD11  | 45:DW:51:LEU:HD11  | 1.89                     | 0.54              |
| 1:AA:1030(B):C:H2' | 1:AA:1030(C):G:C5' | 2.38                     | 0.54              |
| 1:AA:113:G:C2'     | 1:AA:114:U:O5'     | 2.56                     | 0.54              |
| 1:AA:1293:G:O2'    | 1:AA:1294:G:H5'    | 2.07                     | 0.54              |
| 1:AA:1315:U:H2'    | 1:AA:1316:G:O4'    | 2.08                     | 0.54              |
| 1:AA:1393:U:O2'    | 1:AA:1394:A:H3'    | 2.08                     | 0.54              |
| 1:AA:153:C:O2'     | 1:AA:154:C:H5'     | 2.08                     | 0.54              |
| 1:AA:189(B):C:O2'  | 1:AA:189(C):C:H5'  | 2.08                     | 0.54              |
| 1:AA:748:C:O2'     | 1:AA:749:C:OP2     | 2.23                     | 0.54              |
| 1:AA:992:U:HO2'    | 1:AA:993:G:C5'     | 2.19                     | 0.54              |
| 2:AB:122:PHE:HD1   | 2:AB:139:LYS:HZ2   | 1.54                     | 0.54              |
| 7:AG:103:TRP:HA    | 7:AG:106:GLN:HB2   | 1.89                     | 0.54              |
| 13:AM:48:LEU:O     | 13:AM:49:THR:C     | 2.46                     | 0.54              |
| 19:AS:11:VAL:CG2   | 19:AS:16:LEU:HD11  | 2.38                     | 0.54              |
| 23:AW:29:G:C2      | 23:AW:40:C:N3      | 2.76                     | 0.54              |
| 49:B0:53:MET:HA    | 49:B0:58:THR:O     | 2.07                     | 0.54              |
| 55:B6:30:THR:HB    | 55:B6:31:PRO:HD2   | 1.88                     | 0.54              |
| 27:BA:1340:U:H4'   | 27:BA:1341:U:OP2   | 2.08                     | 0.54              |
| 27:BA:200:U:C5'    | 27:BA:200:U:H6     | 2.18                     | 0.54              |
| 27:BA:2023:G:N2    | 27:BA:2024:G:C4    | 2.76                     | 0.54              |
| 27:BA:2483:C:H3'   | 27:BA:2484:G:C5'   | 2.26                     | 0.54              |
| 27:BA:38:A:H1'     | 32:BF:48:THR:O     | 2.07                     | 0.54              |
| 27:BA:636:G:H4'    | 27:BA:638:G:H4'    | 1.90                     | 0.54              |
| 27:BA:959:A:H5''   | 27:BA:959:A:C8     | 2.39                     | 0.54              |
| 27:BA:965:C:H2'    | 27:BA:966:G:C8     | 2.40                     | 0.54              |
| 32:BF:41:LEU:HD21  | 32:BF:184:TYR:CE1  | 2.43                     | 0.54              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 27:BA:444:C:O4'   | 32:BF:49:ALA:HB2    | 2.08                     | 0.54              |
| 33:BG:142:PRO:HG2 | 33:BG:143:GLU:OE1   | 2.07                     | 0.54              |
| 33:BG:120:LEU:O   | 33:BG:181:ARG:HB3   | 2.08                     | 0.54              |
| 39:BQ:35:VAL:HG23 | 39:BQ:100:GLY:O     | 2.06                     | 0.54              |
| 40:BR:28:LEU:CD1  | 40:BR:48:VAL:HG11   | 2.37                     | 0.54              |
| 42:BT:31:SER:CB   | 42:BT:32:TYR:CD2    | 2.90                     | 0.54              |
| 27:BA:2875:C:O2'  | 42:BT:5:ALA:HB2     | 2.08                     | 0.54              |
| 45:BW:85:VAL:CG1  | 45:BW:86:LEU:N      | 2.71                     | 0.54              |
| 47:BY:95:LYS:HZ2  | 47:BY:100:ALA:HB2   | 1.72                     | 0.54              |
| 1:CA:93:G:H2'     | 1:CA:96:U:C5'       | 2.35                     | 0.54              |
| 1:CA:9:G:OP1      | 5:CE:122:GLU:HB2    | 2.08                     | 0.54              |
| 2:CB:101:MET:HA   | 2:CB:108:ILE:HG13   | 1.90                     | 0.54              |
| 2:CB:45:GLN:O     | 2:CB:48:MET:HB3     | 2.08                     | 0.54              |
| 3:CC:94:LEU:HD12  | 3:CC:95:THR:N       | 2.23                     | 0.54              |
| 5:CE:110:LEU:O    | 5:CE:115:VAL:HG23   | 2.07                     | 0.54              |
| 5:CE:80:ILE:CD1   | 5:CE:138:ALA:HB1    | 2.37                     | 0.54              |
| 8:CH:60:ARG:CG    | 8:CH:60:ARG:NH1     | 2.70                     | 0.54              |
| 12:CL:4:ILE:O     | 12:CL:8:VAL:HG23    | 2.08                     | 0.54              |
| 14:CN:7:ILE:CG2   | 14:CN:28:GLY:HA3    | 2.38                     | 0.54              |
| 25:CY:58:A:C2'    | 25:CY:59:U:H5'      | 2.38                     | 0.54              |
| 50:D1:75:GLU:C    | 50:D1:77:ALA:H      | 2.11                     | 0.54              |
| 27:DA:1152:C:H2'  | 27:DA:1153:C:H6     | 1.73                     | 0.54              |
| 27:DA:1379:A:H1'  | 27:DA:1380:G:OP1    | 2.07                     | 0.54              |
| 27:DA:1491:G:OP2  | 27:DA:1494:A:N6     | 2.40                     | 0.54              |
| 27:DA:2537:U:H2'  | 27:DA:2538:C:C6     | 2.42                     | 0.54              |
| 27:DA:2519:U:C4   | 27:DA:2542:A:C2     | 2.95                     | 0.54              |
| 27:DA:2712:U:H2'  | 27:DA:2712(A):A:O5' | 2.07                     | 0.54              |
| 27:DA:491:G:C2'   | 27:DA:492:A:O5'     | 2.56                     | 0.54              |
| 27:DA:706:A:C2'   | 27:DA:707:G:O5'     | 2.55                     | 0.54              |
| 27:DA:729:G:N7    | 30:DD:209:ALA:HB3   | 2.22                     | 0.54              |
| 27:DA:76:C:O2'    | 27:DA:77:C:H5'      | 2.08                     | 0.54              |
| 30:DD:143:HIS:HA  | 30:DD:156:ALA:CB    | 2.37                     | 0.54              |
| 30:DD:30:GLU:HG3  | 30:DD:63:ARG:NH2    | 2.22                     | 0.54              |
| 33:DG:16:ARG:O    | 33:DG:20:ILE:HG13   | 2.08                     | 0.54              |
| 27:DA:2310:A:N6   | 33:DG:75:LYS:HE2    | 2.23                     | 0.54              |
| 34:DH:35:VAL:HG11 | 34:DH:71:LEU:HG     | 1.90                     | 0.54              |
| 35:DI:45:LYS:O    | 35:DI:48:GLU:N      | 2.39                     | 0.54              |
| 38:DP:112:LEU:O   | 38:DP:112:LEU:HD13  | 2.08                     | 0.54              |
| 38:DP:47:ASP:HB3  | 38:DP:48:PRO:C      | 2.28                     | 0.54              |
| 41:DS:30:ARG:HB3  | 41:DS:89:ARG:NH2    | 2.23                     | 0.54              |
| 41:DS:98:VAL:O    | 41:DS:98:VAL:HG13   | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DT:38:ASN:ND2   | 42:DT:38:ASN:O     | 2.41                     | 0.54              |
| 43:DU:62:ILE:HG22  | 43:DU:63:VAL:N     | 2.22                     | 0.54              |
| 44:DV:81:TYR:CE2   | 44:DV:83:ARG:CZ    | 2.91                     | 0.54              |
| 48:DZ:4:LEU:CD1    | 48:DZ:5:LYS:H      | 2.17                     | 0.54              |
| 1:AA:1465:C:H2'    | 1:AA:1466:C:O4'    | 2.07                     | 0.54              |
| 1:AA:163:C:H2'     | 1:AA:164:U:C6      | 2.42                     | 0.54              |
| 1:AA:175:C:H2'     | 1:AA:176:C:C6      | 2.43                     | 0.54              |
| 1:AA:321:A:N1      | 1:AA:333:G:C2      | 2.76                     | 0.54              |
| 1:AA:344:A:H2'     | 1:AA:346:G:O6      | 2.07                     | 0.54              |
| 1:AA:609:A:H2'     | 1:AA:610:G:H5'     | 1.87                     | 0.54              |
| 1:AA:701:C:H1'     | 1:AA:703:G:C2      | 2.43                     | 0.54              |
| 1:AA:782:A:H2'     | 1:AA:783:C:H5'     | 1.90                     | 0.54              |
| 2:AB:100:GLY:O     | 2:AB:101:MET:C     | 2.45                     | 0.54              |
| 2:AB:75:LYS:HD3    | 2:AB:78:GLN:HB2    | 1.90                     | 0.54              |
| 4:AD:25:ARG:HG2    | 4:AD:25:ARG:NH1    | 2.21                     | 0.54              |
| 8:AH:34:GLU:O      | 8:AH:38:ILE:HG13   | 2.07                     | 0.54              |
| 9:AI:5:TYR:HA      | 9:AI:17:VAL:O      | 2.07                     | 0.54              |
| 10:AJ:53:PRO:HA    | 14:AN:41:ARG:HH21  | 1.72                     | 0.54              |
| 11:AK:12:ARG:HG3   | 11:AK:13:GLN:N     | 2.23                     | 0.54              |
| 12:AL:114:ARG:HD2  | 12:AL:119:THR:CG2  | 2.38                     | 0.54              |
| 12:AL:25:LYS:HE3   | 12:AL:30:ARG:HH22  | 1.72                     | 0.54              |
| 16:AP:8:ARG:O      | 16:AP:9:PHE:CG     | 2.60                     | 0.54              |
| 17:AQ:26:GLN:NE2   | 17:AQ:37:LYS:HG2   | 2.23                     | 0.54              |
| 19:AS:18:LYS:HD2   | 19:AS:22:LEU:CD2   | 2.37                     | 0.54              |
| 20:AT:13:LEU:C     | 20:AT:13:LEU:HD12  | 2.27                     | 0.54              |
| 25:AY:14:A:H5''    | 25:AY:15:G:N7      | 2.22                     | 0.54              |
| 27:BA:1032:A:OP1   | 58:B9:8:LYS:HE3    | 2.08                     | 0.54              |
| 27:BA:1963:U:C2'   | 27:BA:1963:U:O2    | 2.55                     | 0.54              |
| 27:BA:2710:C:O2'   | 27:BA:2711:A:H5'   | 2.07                     | 0.54              |
| 27:BA:995:C:O2     | 36:BN:4:TYR:OH     | 2.26                     | 0.54              |
| 30:BD:186:HIS:NE2  | 30:BD:188:GLU:HG2  | 2.23                     | 0.54              |
| 30:BD:227:ASN:O    | 30:BD:234:GLY:HA3  | 2.08                     | 0.54              |
| 33:BG:101:ILE:HG12 | 33:BG:105:LYS:CE   | 2.32                     | 0.54              |
| 33:BG:114:ILE:HG12 | 33:BG:140:ILE:HD13 | 1.90                     | 0.54              |
| 34:BH:89:ILE:O     | 34:BH:90:LYS:C     | 2.46                     | 0.54              |
| 36:BN:123:TYR:OH   | 36:BN:130:HIS:CE1  | 2.61                     | 0.54              |
| 43:BU:114:LYS:O    | 43:BU:117:GLN:HB2  | 2.07                     | 0.54              |
| 43:BU:92:ARG:HH21  | 44:BV:11:GLN:H     | 1.55                     | 0.54              |
| 45:BW:12:ILE:O     | 45:BW:101:SER:OG   | 2.23                     | 0.54              |
| 47:BY:88:LYS:NZ    | 47:BY:93:GLY:CA    | 2.67                     | 0.54              |
| 47:BY:95:LYS:HG2   | 47:BY:99:CYS:O     | 2.07                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:BY:96:ILE:HD12  | 47:BY:99:CYS:HB2  | 1.90                     | 0.54              |
| 48:BZ:99:VAL:O     | 48:BZ:122:ASP:HA  | 2.08                     | 0.54              |
| 48:BZ:164:VAL:HG11 | 48:BZ:168:GLU:HB2 | 1.89                     | 0.54              |
| 1:CA:417:C:O2'     | 1:CA:418:C:H5'    | 2.07                     | 0.54              |
| 1:CA:498:U:O2'     | 1:CA:499:A:O5'    | 2.25                     | 0.54              |
| 1:CA:686:U:C2'     | 1:CA:686:U:O2     | 2.55                     | 0.54              |
| 2:CB:106:LYS:HG2   | 2:CB:106:LYS:O    | 2.08                     | 0.54              |
| 1:CA:1191:A:H5''   | 3:CC:4:LYS:HZ3    | 1.70                     | 0.54              |
| 4:CD:171:GLY:HA3   | 4:CD:173:TRP:CZ3  | 2.43                     | 0.54              |
| 7:CG:127:ALA:O     | 7:CG:130:GLY:N    | 2.40                     | 0.54              |
| 12:CL:25:LYS:C     | 12:CL:27:ALA:N    | 2.61                     | 0.54              |
| 12:CL:57:LEU:C     | 12:CL:59:SER:H    | 2.10                     | 0.54              |
| 13:CM:116:THR:O    | 13:CM:117:VAL:CB  | 2.56                     | 0.54              |
| 13:CM:48:LEU:HB2   | 13:CM:52:GLU:HB3  | 1.89                     | 0.54              |
| 13:CM:6:GLY:O      | 13:CM:7:VAL:CG2   | 2.56                     | 0.54              |
| 14:CN:9:LYS:HA     | 14:CN:12:ARG:CZ   | 2.38                     | 0.54              |
| 23:CW:10:G:C2      | 23:CW:25:A:H1'    | 2.42                     | 0.54              |
| 54:D5:25:LEU:CD2   | 54:D5:26:THR:N    | 2.70                     | 0.54              |
| 57:D8:38:GLY:O     | 57:D8:42:ARG:CB   | 2.55                     | 0.54              |
| 27:DA:1009:A:H5'   | 27:DA:1009:A:C8   | 2.42                     | 0.54              |
| 27:DA:1042:G:H5''  | 27:DA:1043:C:C5   | 2.43                     | 0.54              |
| 27:DA:1301:A:C4'   | 27:DA:1302:A:OP1  | 2.55                     | 0.54              |
| 27:DA:2386:C:H4'   | 49:D0:55:ARG:O    | 2.07                     | 0.54              |
| 27:DA:2747:G:N2    | 27:DA:2748:A:H62  | 2.05                     | 0.54              |
| 27:DA:407:G:N2     | 27:DA:421:U:C2    | 2.76                     | 0.54              |
| 27:DA:599:G:O2'    | 27:DA:600:G:H5'   | 2.06                     | 0.54              |
| 27:DA:65:C:H2'     | 27:DA:66:C:C6     | 2.43                     | 0.54              |
| 27:DA:902:C:H2'    | 27:DA:903:C:C6    | 2.42                     | 0.54              |
| 30:DD:94:LEU:CD2   | 30:DD:95:LEU:N    | 2.71                     | 0.54              |
| 38:DP:30:THR:HG22  | 38:DP:31:ALA:H    | 1.71                     | 0.54              |
| 46:DX:35:THR:HG22  | 46:DX:37:THR:H    | 1.73                     | 0.54              |
| 1:AA:1149:C:H2'    | 1:AA:1150:U:H6    | 1.73                     | 0.54              |
| 1:AA:1285:A:O2'    | 1:AA:1286:A:OP2   | 2.24                     | 0.54              |
| 1:AA:1458:G:O2'    | 1:AA:1459:C:H5'   | 2.08                     | 0.54              |
| 1:AA:184:G:O2'     | 1:AA:185:A:H5'    | 2.06                     | 0.54              |
| 6:AF:18:GLN:O      | 6:AF:22:GLU:HG2   | 2.08                     | 0.54              |
| 10:AJ:17:ASP:OD1   | 10:AJ:70:ARG:NH1  | 2.41                     | 0.54              |
| 14:AN:13:THR:N     | 14:AN:14:PRO:CD   | 2.69                     | 0.54              |
| 16:AP:3:LYS:HG2    | 16:AP:65:GLN:O    | 2.08                     | 0.54              |
| 19:AS:50:ALA:HB1   | 19:AS:57:HIS:HB3  | 1.90                     | 0.54              |
| 21:AU:8:THR:O      | 21:AU:12:LYS:HB2  | 2.07                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:397:G:OP1    | 50:B1:44:PRO:HA   | 2.08                     | 0.54              |
| 50:B1:73:LEU:C     | 50:B1:75:GLU:N    | 2.61                     | 0.54              |
| 51:B2:16:LEU:O     | 51:B2:17:SER:HB3  | 2.06                     | 0.54              |
| 46:BX:8:ILE:O      | 51:B2:36:ARG:NH2  | 2.40                     | 0.54              |
| 52:B3:12:PRO:O     | 52:B3:15:TYR:HB2  | 2.08                     | 0.54              |
| 27:BA:1114:G:H2'   | 27:BA:1115:G:H5'' | 1.89                     | 0.54              |
| 27:BA:991:C:O2     | 27:BA:1164:G:C2   | 2.60                     | 0.54              |
| 27:BA:1931:U:H2'   | 27:BA:1932:A:H8   | 1.73                     | 0.54              |
| 27:BA:216:A:H2'    | 27:BA:217:G:H8    | 1.72                     | 0.54              |
| 27:BA:2423:U:H4'   | 27:BA:2425:A:C8   | 2.43                     | 0.54              |
| 27:BA:2562:U:O2'   | 27:BA:2563:U:H5'  | 2.08                     | 0.54              |
| 27:BA:2636:U:O2'   | 31:BE:44:TYR:HE1  | 1.91                     | 0.54              |
| 27:BA:2694:G:H2'   | 27:BA:2695:C:O5'  | 2.08                     | 0.54              |
| 27:BA:363(B):G:C2' | 27:BA:363(B):G:N3 | 2.68                     | 0.54              |
| 27:BA:425:G:H2'    | 27:BA:426:C:C6    | 2.41                     | 0.54              |
| 27:BA:729:G:O2'    | 27:BA:763:G:H4'   | 2.08                     | 0.54              |
| 27:BA:853:G:O2'    | 27:BA:854:G:H5'   | 2.08                     | 0.54              |
| 27:BA:971:C:H2'    | 27:BA:972:G:C5'   | 2.38                     | 0.54              |
| 28:BB:111:G:O2'    | 28:BB:112:U:H5'   | 2.07                     | 0.54              |
| 31:BE:34:VAL:HG22  | 31:BE:48:GLN:HE21 | 1.72                     | 0.54              |
| 27:BA:797:C:OP2    | 32:BF:62:ARG:HG3  | 2.08                     | 0.54              |
| 27:BA:2310:A:N7    | 33:BG:75:LYS:HE2  | 2.23                     | 0.54              |
| 27:BA:1138:G:N3    | 36:BN:106:MET:CE  | 2.71                     | 0.54              |
| 39:BQ:12:GLN:HE21  | 39:BQ:73:PRO:CD   | 2.21                     | 0.54              |
| 39:BQ:4:PRO:C      | 39:BQ:5:ARG:HG3   | 2.28                     | 0.54              |
| 48:BZ:143:LEU:HD12 | 48:BZ:147:ASP:HB3 | 1.89                     | 0.54              |
| 1:CA:1049:U:O2'    | 1:CA:1050:G:OP2   | 2.25                     | 0.54              |
| 1:CA:1139:G:H4'    | 1:CA:1140:C:O5'   | 2.06                     | 0.54              |
| 1:CA:1176:A:H2'    | 1:CA:1177:G:O4'   | 2.07                     | 0.54              |
| 1:CA:1319:A:OP2    | 19:CS:5:LEU:HD23  | 2.07                     | 0.54              |
| 1:CA:243:A:N6      | 1:CA:281:G:H1'    | 2.23                     | 0.54              |
| 1:CA:590:C:O2'     | 1:CA:591:U:H5'    | 2.08                     | 0.54              |
| 2:CB:200:ILE:O     | 2:CB:201:ILE:HD13 | 2.07                     | 0.54              |
| 2:CB:97:TRP:HH2    | 2:CB:176:GLU:OE1  | 1.90                     | 0.54              |
| 4:CD:100:ARG:O     | 4:CD:102:ASP:N    | 2.40                     | 0.54              |
| 8:CH:42:GLU:HG3    | 8:CH:109:ILE:CD1  | 2.33                     | 0.54              |
| 8:CH:90:GLY:O      | 8:CH:91:ARG:CB    | 2.55                     | 0.54              |
| 12:CL:33:VAL:O     | 12:CL:55:VAL:HG13 | 2.08                     | 0.54              |
| 15:CO:10:LYS:HE3   | 15:CO:11:VAL:HG23 | 1.90                     | 0.54              |
| 15:CO:29:VAL:HG12  | 15:CO:30:ALA:N    | 2.22                     | 0.54              |
| 17:CQ:60:ILE:O     | 17:CQ:71:PHE:CD1  | 2.60                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:84:ILE:N     | 19:CS:66:MET:HE1   | 2.22                     | 0.54              |
| 20:CT:49:ALA:HB1   | 20:CT:100:ILE:HD13 | 1.89                     | 0.54              |
| 24:CX:28:C:H42     | 24:CX:42:G:H1      | 1.55                     | 0.54              |
| 25:CY:17:G:N2      | 25:CY:54:U:H1'     | 2.19                     | 0.54              |
| 52:D3:1:MET:O      | 52:D3:2:PRO:O      | 2.26                     | 0.54              |
| 55:D6:10:LEU:N     | 55:D6:10:LEU:CD2   | 2.69                     | 0.54              |
| 55:D6:40:CYS:SG    | 55:D6:45:LYS:NZ    | 2.70                     | 0.54              |
| 57:D8:6:THR:CG2    | 57:D8:63:PRO:HG3   | 2.37                     | 0.54              |
| 27:DA:813:U:C2     | 27:DA:1195:G:N2    | 2.76                     | 0.54              |
| 27:DA:1515:G:O2'   | 27:DA:1516:C:H5'   | 2.07                     | 0.54              |
| 27:DA:1679:U:H2'   | 27:DA:1680:U:C6    | 2.42                     | 0.54              |
| 27:DA:1711:C:O2'   | 27:DA:1712:C:H5'   | 2.08                     | 0.54              |
| 27:DA:1911:U:O2'   | 27:DA:1912:A:H5''  | 2.08                     | 0.54              |
| 27:DA:2023:G:O2'   | 27:DA:2024:G:C8    | 2.60                     | 0.54              |
| 27:DA:2453:A:H2'   | 27:DA:2454:G:H8    | 1.71                     | 0.54              |
| 27:DA:2061:G:C8    | 27:DA:2501:C:H1'   | 2.43                     | 0.54              |
| 30:DD:138:VAL:HG12 | 30:DD:168:ARG:HE   | 1.73                     | 0.54              |
| 34:DH:125:VAL:HG13 | 34:DH:131:VAL:HG22 | 1.90                     | 0.54              |
| 35:DI:133:HIS:ND1  | 35:DI:134:PRO:CD   | 2.70                     | 0.54              |
| 42:DT:101:PHE:O    | 42:DT:103:ARG:N    | 2.41                     | 0.54              |
| 44:DV:21:ARG:HB3   | 44:DV:91:TYR:HB2   | 1.90                     | 0.54              |
| 45:DW:84:ARG:HG3   | 45:DW:98:LYS:NZ    | 2.23                     | 0.54              |
| 1:AA:1161:C:H2'    | 1:AA:1162:C:H6     | 1.72                     | 0.54              |
| 1:AA:1047:G:H1     | 1:AA:1210:C:H42    | 1.54                     | 0.54              |
| 1:AA:132:C:O2'     | 1:AA:133:U:H5'     | 2.08                     | 0.54              |
| 1:AA:197:A:N6      | 1:AA:221:C:H5'     | 2.23                     | 0.54              |
| 1:AA:372:C:H42     | 1:AA:389:A:H62     | 1.54                     | 0.54              |
| 1:AA:524:G:H8      | 1:AA:524:G:OP1     | 1.91                     | 0.54              |
| 1:AA:577:G:O2'     | 1:AA:578:C:H5'     | 2.06                     | 0.54              |
| 2:AB:167:PRO:HG2   | 2:AB:192:SER:CB    | 2.37                     | 0.54              |
| 2:AB:61:LEU:HD23   | 2:AB:68:ILE:HD11   | 1.88                     | 0.54              |
| 2:AB:91:PRO:HA     | 2:AB:154:LEU:HD12  | 1.90                     | 0.54              |
| 3:AC:84:ILE:O      | 3:AC:88:ARG:HG3    | 2.08                     | 0.54              |
| 7:AG:153:HIS:CG    | 11:AK:58:PRO:HG3   | 2.42                     | 0.54              |
| 51:B2:13:ALA:C     | 51:B2:15:LYS:H     | 2.10                     | 0.54              |
| 52:B3:24:LYS:O     | 52:B3:27:GLY:N     | 2.40                     | 0.54              |
| 55:B6:40:CYS:CB    | 55:B6:46:HIS:HB3   | 2.38                     | 0.54              |
| 27:BA:125:G:C6     | 56:B7:10:ARG:NE    | 2.74                     | 0.54              |
| 38:BP:64:LYS:HD2   | 57:B8:25:MET:SD    | 2.48                     | 0.54              |
| 27:BA:577:G:O2'    | 27:BA:1254:A:OP1   | 2.26                     | 0.54              |
| 27:BA:1931:U:C6    | 27:BA:1931:U:C5'   | 2.90                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:1983:C:O2'   | 27:BA:1984:G:H5'  | 2.08                     | 0.54              |
| 27:BA:2006:C:H2'   | 27:BA:2007:C:H6   | 1.73                     | 0.54              |
| 27:BA:2648:C:H2'   | 27:BA:2649:U:H6   | 1.72                     | 0.54              |
| 27:BA:271(G):C:H2' | 27:BA:271(H):G:C8 | 2.41                     | 0.54              |
| 27:BA:27:G:O2'     | 27:BA:28:A:H8     | 1.91                     | 0.54              |
| 27:BA:752:A:C5     | 27:BA:1781:C:O4'  | 2.61                     | 0.54              |
| 27:BA:803:U:O2'    | 27:BA:804:A:H5'   | 2.08                     | 0.54              |
| 29:BC:36:LYS:HD3   | 29:BC:37:PHE:N    | 2.23                     | 0.54              |
| 29:BC:42:GLU:H     | 29:BC:213:TYR:N   | 2.02                     | 0.54              |
| 29:BC:87:GLU:HG2   | 29:BC:92:ASP:O    | 2.08                     | 0.54              |
| 33:BG:86:MET:HB2   | 33:BG:87:PRO:HD3  | 1.89                     | 0.54              |
| 33:BG:66:GLN:HE21  | 33:BG:98:ARG:HG3  | 1.72                     | 0.54              |
| 41:BS:88:ASP:CG    | 41:BS:89:ARG:N    | 2.61                     | 0.54              |
| 42:BT:27:THR:HA    | 42:BT:87:ASP:HB2  | 1.88                     | 0.54              |
| 44:BV:28:GLU:HB3   | 44:BV:29:PRO:CD   | 2.38                     | 0.54              |
| 45:BW:33:ARG:HG3   | 45:BW:33:ARG:NH1  | 2.23                     | 0.54              |
| 47:BY:90:LEU:HD12  | 47:BY:91:GLU:N    | 2.13                     | 0.54              |
| 1:CA:1005:A:H2'    | 1:CA:1006:C:H5'   | 1.90                     | 0.54              |
| 1:CA:919:A:O2'     | 1:CA:1080:A:N1    | 2.38                     | 0.54              |
| 1:CA:1109:C:O2'    | 1:CA:1110:A:H5'   | 2.08                     | 0.54              |
| 1:CA:242:C:C2'     | 1:CA:243:A:H5'    | 2.38                     | 0.54              |
| 1:CA:62:U:H3       | 1:CA:105:G:H1     | 1.55                     | 0.54              |
| 1:CA:750:G:H21     | 15:CO:23:GLY:HA3  | 1.72                     | 0.54              |
| 1:CA:958:A:C8      | 19:CS:55:LYS:HD2  | 2.42                     | 0.54              |
| 2:CB:105:PHE:C     | 2:CB:107:THR:H    | 2.10                     | 0.54              |
| 2:CB:16:HIS:HB3    | 2:CB:210:SER:OG   | 2.08                     | 0.54              |
| 4:CD:79:PHE:HA     | 4:CD:93:PHE:CE2   | 2.43                     | 0.54              |
| 5:CE:94:ALA:HB1    | 5:CE:98:THR:HB    | 1.90                     | 0.54              |
| 10:CJ:61:GLU:OE1   | 14:CN:58:LYS:HE2  | 2.08                     | 0.54              |
| 10:CJ:82:ILE:CG2   | 10:CJ:82:ILE:O    | 2.56                     | 0.54              |
| 12:CL:80:VAL:HG12  | 12:CL:81:LEU:N    | 2.18                     | 0.54              |
| 12:CL:83:ARG:N     | 12:CL:96:HIS:O    | 2.35                     | 0.54              |
| 13:CM:48:LEU:HG    | 13:CM:53:VAL:HG23 | 1.90                     | 0.54              |
| 17:CQ:50:LYS:O     | 17:CQ:52:LYS:HD2  | 2.08                     | 0.54              |
| 19:CS:45:VAL:HA    | 19:CS:62:ILE:HG23 | 1.88                     | 0.54              |
| 20:CT:8:ARG:HG3    | 20:CT:8:ARG:NH1   | 2.22                     | 0.54              |
| 49:D0:32:ARG:H     | 49:D0:35:ASN:ND2  | 2.05                     | 0.54              |
| 50:D1:51:VAL:O     | 50:D1:57:GLU:O    | 2.25                     | 0.54              |
| 54:D5:59:GLU:O     | 54:D5:60:VAL:HG23 | 2.07                     | 0.54              |
| 58:D9:5:ALA:O      | 58:D9:36:GLN:HG3  | 2.08                     | 0.54              |
| 27:DA:1164:G:C2    | 27:DA:1165:U:C2   | 2.96                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1446:C:O2'   | 27:DA:1447:G:H5'   | 2.08                     | 0.54              |
| 27:DA:1665:A:C2'   | 27:DA:1666:G:H5'   | 2.38                     | 0.54              |
| 27:DA:2131:G:OP1   | 27:DA:2132:U:H3'   | 2.08                     | 0.54              |
| 27:DA:2461:C:C5    | 27:DA:2462:U:C5    | 2.95                     | 0.54              |
| 27:DA:36:G:N3      | 27:DA:450:G:O2'    | 2.41                     | 0.54              |
| 27:DA:483:A:N7     | 27:DA:497:A:H2     | 2.06                     | 0.54              |
| 27:DA:582:G:H2'    | 27:DA:583:G:H8     | 1.71                     | 0.54              |
| 27:DA:828:U:H4'    | 27:DA:831:G:N1     | 2.23                     | 0.54              |
| 28:DB:110:G:C2'    | 28:DB:111:G:H5'    | 2.38                     | 0.54              |
| 30:DD:158:ALA:O    | 30:DD:196:VAL:HG11 | 2.08                     | 0.54              |
| 30:DD:144:ALA:HB3  | 30:DD:192:THR:HG23 | 1.90                     | 0.54              |
| 31:DE:179:GLU:CB   | 31:DE:181:LEU:HD13 | 2.28                     | 0.54              |
| 34:DH:12:PRO:CG    | 34:DH:49:VAL:HA    | 2.28                     | 0.54              |
| 35:DI:109:ILE:HD12 | 35:DI:109:ILE:N    | 2.23                     | 0.54              |
| 27:DA:587:C:C6     | 38:DP:33:ARG:NH1   | 2.76                     | 0.54              |
| 39:DQ:130:LYS:HG3  | 39:DQ:131:ILE:N    | 2.22                     | 0.54              |
| 40:DR:33:ARG:HG3   | 40:DR:115:GLU:HB3  | 1.90                     | 0.54              |
| 41:DS:96:GLY:O     | 41:DS:98:VAL:HG12  | 2.08                     | 0.54              |
| 43:DU:5:LYS:CG     | 43:DU:7:GLY:H      | 2.21                     | 0.54              |
| 43:DU:91:ASP:C     | 43:DU:92:ARG:HD3   | 2.27                     | 0.54              |
| 44:DV:52:VAL:O     | 44:DV:52:VAL:HG13  | 2.07                     | 0.54              |
| 27:DA:84:A:C5'     | 47:DY:9:LYS:HZ1    | 2.17                     | 0.54              |
| 1:AA:1043:C:H2'    | 1:AA:1044:A:H8     | 1.69                     | 0.54              |
| 1:AA:1064:G:H1'    | 1:AA:1066:C:C5     | 2.43                     | 0.54              |
| 1:AA:1299:A:N3     | 1:AA:1299:A:H5'    | 2.23                     | 0.54              |
| 1:AA:1463:C:O2'    | 1:AA:1464:G:H5'    | 2.08                     | 0.54              |
| 1:AA:163:C:O2'     | 1:AA:164:U:H5'     | 2.07                     | 0.54              |
| 1:AA:292:G:N7      | 1:AA:293:G:H1'     | 2.22                     | 0.54              |
| 1:AA:803:G:H2'     | 1:AA:804:U:H6      | 1.73                     | 0.54              |
| 1:AA:806:C:O2'     | 1:AA:807:A:H5'     | 2.07                     | 0.54              |
| 1:AA:818:G:H3'     | 1:AA:819:A:C5'     | 2.38                     | 0.54              |
| 4:AD:128:VAL:O     | 4:AD:130:GLY:N     | 2.41                     | 0.54              |
| 4:AD:52:SER:O      | 4:AD:55:ALA:N      | 2.41                     | 0.54              |
| 6:AF:14:LEU:HD22   | 6:AF:18:GLN:HE21   | 1.73                     | 0.54              |
| 8:AH:34:GLU:CB     | 8:AH:118:VAL:HG21  | 2.25                     | 0.54              |
| 10:AJ:22:LYS:C     | 10:AJ:22:LYS:HD2   | 2.28                     | 0.54              |
| 13:AM:97:PRO:HB2   | 13:AM:101:GLN:NE2  | 2.23                     | 0.54              |
| 15:AO:39:LEU:C     | 15:AO:41:GLU:N     | 2.60                     | 0.54              |
| 23:AW:38:U:H2'     | 23:AW:39:C:C6      | 2.43                     | 0.54              |
| 49:B0:41:ARG:H     | 49:B0:41:ARG:CD    | 2.21                     | 0.54              |
| 55:B6:32:ASN:CG    | 55:B6:33:LYS:N     | 2.61                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:1358:G:H8   | 27:BA:1358:G:O5'  | 1.90                     | 0.54              |
| 27:BA:1627:G:C2   | 27:BA:1628:G:N7   | 2.76                     | 0.54              |
| 27:BA:1641:A:N6   | 27:BA:1642:G:C2   | 2.76                     | 0.54              |
| 27:BA:1916:A:H3'  | 27:BA:1917:U:C6   | 2.41                     | 0.54              |
| 27:BA:2187:G:H5'  | 27:BA:2188:C:OP2  | 2.08                     | 0.54              |
| 27:BA:2420:C:O5'  | 27:BA:2420:C:H6   | 1.91                     | 0.54              |
| 27:BA:2850:A:C2   | 27:BA:2851:A:C4   | 2.96                     | 0.54              |
| 27:BA:416:C:H2'   | 27:BA:416:C:O2    | 2.07                     | 0.54              |
| 27:BA:608:A:OP1   | 32:BF:100:THR:CG2 | 2.51                     | 0.54              |
| 31:BE:45:THR:O    | 31:BE:46:ALA:HB2  | 2.08                     | 0.54              |
| 34:BH:43:VAL:CG1  | 34:BH:53:GLU:H    | 2.19                     | 0.54              |
| 34:BH:8:PRO:O     | 34:BH:9:ILE:CB    | 2.56                     | 0.54              |
| 34:BH:92:ILE:CG2  | 34:BH:93:GLY:N    | 2.60                     | 0.54              |
| 35:BI:120:ILE:O   | 35:BI:121:LYS:HB3 | 2.08                     | 0.54              |
| 36:BN:15:LEU:HB3  | 36:BN:136:GLU:HG2 | 1.89                     | 0.54              |
| 37:BO:6:THR:O     | 37:BO:20:MET:HA   | 2.09                     | 0.54              |
| 38:BP:130:PHE:CD2 | 38:BP:130:PHE:N   | 2.76                     | 0.54              |
| 40:BR:29:LEU:HD11 | 40:BR:48:VAL:HG12 | 1.89                     | 0.54              |
| 40:BR:53:HIS:CD2  | 40:BR:94:TYR:OH   | 2.60                     | 0.54              |
| 43:BU:65:ILE:O    | 43:BU:69:CYS:SG   | 2.64                     | 0.54              |
| 1:CA:1118:C:O2'   | 1:CA:1119:C:H5'   | 2.08                     | 0.54              |
| 1:CA:1143:G:H2'   | 1:CA:1144:G:C8    | 2.43                     | 0.54              |
| 1:CA:106:C:O2     | 1:CA:379:C:H4'    | 2.08                     | 0.54              |
| 1:CA:544:G:H2'    | 1:CA:545:C:C6     | 2.43                     | 0.54              |
| 1:CA:563:A:N3     | 1:CA:563:A:H2'    | 2.22                     | 0.54              |
| 1:CA:60:A:OP1     | 1:CA:111:G:N2     | 2.38                     | 0.54              |
| 1:CA:741:G:H2'    | 1:CA:742:G:C8     | 2.43                     | 0.54              |
| 3:CC:28:GLN:O     | 3:CC:32:LEU:HG    | 2.07                     | 0.54              |
| 4:CD:76:ARG:O     | 4:CD:77:ASN:C     | 2.46                     | 0.54              |
| 7:CG:78:ARG:CG    | 7:CG:79:ARG:N     | 2.65                     | 0.54              |
| 5:CE:78:HIS:ND1   | 8:CH:107:LEU:HD13 | 2.22                     | 0.54              |
| 9:CI:26:VAL:CG2   | 9:CI:61:ALA:HB3   | 2.32                     | 0.54              |
| 10:CJ:63:PHE:HA   | 14:CN:59:ALA:HB2  | 1.89                     | 0.54              |
| 20:CT:49:ALA:HB1  | 20:CT:100:ILE:CD1 | 2.38                     | 0.54              |
| 24:CX:1:C:H1'     | 49:D0:5:LYS:HE2   | 1.90                     | 0.54              |
| 54:D5:31:VAL:HB   | 54:D5:32:PRO:HD3  | 1.90                     | 0.54              |
| 27:DA:243:U:OP1   | 57:D8:6:THR:CG2   | 2.55                     | 0.54              |
| 27:DA:1042:G:N3   | 27:DA:1042:G:H2'  | 2.23                     | 0.54              |
| 27:DA:1310:G:OP2  | 56:D7:9:ARG:NE    | 2.41                     | 0.54              |
| 27:DA:1655:A:H4'  | 31:DE:115:GLY:N   | 2.23                     | 0.54              |
| 27:DA:2356:C:H5'' | 49:D0:20:ARG:HG2  | 1.89                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:2682:U:O4'   | 31:DE:12:THR:HA   | 2.08                     | 0.54              |
| 27:DA:291:C:H2'    | 27:DA:292:C:C6    | 2.40                     | 0.54              |
| 27:DA:469:G:O2'    | 27:DA:470:A:H5''  | 2.08                     | 0.54              |
| 27:DA:19:C:H42     | 27:DA:521:G:H1    | 1.54                     | 0.54              |
| 27:DA:542:C:C2'    | 27:DA:543:C:OP1   | 2.55                     | 0.54              |
| 27:DA:542:C:H2'    | 27:DA:543:C:OP1   | 2.08                     | 0.54              |
| 27:DA:749:C:O2     | 27:DA:1618:A:H2'  | 2.08                     | 0.54              |
| 27:DA:817:C:H4'    | 27:DA:932:G:C6    | 2.43                     | 0.54              |
| 27:DA:861:A:C2     | 27:DA:862:G:H1'   | 2.42                     | 0.54              |
| 27:DA:965:C:C2'    | 27:DA:966:G:H5'   | 2.38                     | 0.54              |
| 27:DA:919:G:C5'    | 28:DB:81:G:H1'    | 2.35                     | 0.54              |
| 29:DC:62:VAL:O     | 29:DC:64:LEU:N    | 2.41                     | 0.54              |
| 31:DE:11:MET:HB2   | 31:DE:24:THR:HA   | 1.89                     | 0.54              |
| 33:DG:11:TYR:CE2   | 33:DG:16:ARG:HG2  | 2.43                     | 0.54              |
| 36:DN:27:ALA:HB3   | 36:DN:106:MET:HE1 | 1.89                     | 0.54              |
| 36:DN:118:LYS:O    | 36:DN:120:LEU:N   | 2.41                     | 0.54              |
| 36:DN:11:PRO:HB3   | 36:DN:51:PHE:CE1  | 2.42                     | 0.54              |
| 36:DN:11:PRO:HB3   | 36:DN:51:PHE:HD1  | 1.71                     | 0.54              |
| 37:DO:88:ASN:HD21  | 37:DO:92:GLU:HB2  | 1.72                     | 0.54              |
| 39:DQ:27:VAL:HG23  | 39:DQ:137:TYR:CE1 | 2.43                     | 0.54              |
| 41:DS:101:LEU:HD13 | 41:DS:101:LEU:H   | 1.71                     | 0.54              |
| 44:DV:64:HIS:ND1   | 44:DV:92:THR:HG22 | 2.23                     | 0.54              |
| 27:DA:495:G:H21    | 45:DW:61:ASN:CG   | 2.11                     | 0.54              |
| 46:DX:4:ALA:HB3    | 46:DX:5:TYR:HD1   | 1.72                     | 0.54              |
| 48:DZ:54:HIS:CE1   | 48:DZ:134:GLU:HG3 | 2.43                     | 0.54              |
| 48:DZ:39:ASP:OD2   | 48:DZ:42:GLU:HG3  | 2.07                     | 0.54              |
| 1:AA:107:G:H5''    | 1:AA:108:G:OP2    | 2.08                     | 0.53              |
| 1:AA:1137:C:C4'    | 1:AA:1138:G:N2    | 2.68                     | 0.53              |
| 2:AB:149:LEU:O     | 2:AB:150:SER:C    | 2.46                     | 0.53              |
| 3:AC:95:THR:O      | 3:AC:97:LYS:N     | 2.42                     | 0.53              |
| 4:AD:52:SER:O      | 4:AD:55:ALA:HB3   | 2.08                     | 0.53              |
| 8:AH:53:VAL:O      | 8:AH:54:ASP:C     | 2.47                     | 0.53              |
| 9:AI:26:VAL:HG13   | 9:AI:61:ALA:CB    | 2.37                     | 0.53              |
| 23:AW:4:G:H2'      | 23:AW:5:G:C5'     | 2.39                     | 0.53              |
| 52:B3:52:HIS:ND1   | 52:B3:53:LEU:HG   | 2.24                     | 0.53              |
| 58:B9:32:HIS:O     | 58:B9:34:GLN:HG3  | 2.09                     | 0.53              |
| 27:BA:1055:G:H2'   | 27:BA:1108:U:O4'  | 2.08                     | 0.53              |
| 27:BA:1165:U:O2'   | 27:BA:1166:C:H5'  | 2.08                     | 0.53              |
| 27:BA:1359:A:N6    | 27:BA:1372:U:H3   | 2.02                     | 0.53              |
| 27:BA:1491:G:OP2   | 27:BA:1494:A:N6   | 2.38                     | 0.53              |
| 27:BA:16:G:O2'     | 27:BA:17:G:H5'    | 2.07                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2445:G:O2'   | 27:BA:2446:G:H5'   | 2.09                     | 0.53              |
| 27:BA:2510:C:O2'   | 27:BA:2511:U:H5'   | 2.08                     | 0.53              |
| 27:BA:2655:G:O2'   | 27:BA:2656:U:P     | 2.66                     | 0.53              |
| 27:BA:2792:G:HO2'  | 27:BA:2793:G:H8    | 0.68                     | 0.53              |
| 27:BA:2809:A:C6    | 27:BA:2892:A:H1'   | 2.43                     | 0.53              |
| 27:BA:863:A:O2'    | 27:BA:864:G:H5'    | 2.08                     | 0.53              |
| 32:BF:40:GLN:NE2   | 32:BF:184:TYR:CB   | 2.71                     | 0.53              |
| 32:BF:95:ARG:NH2   | 32:BF:97:TYR:OH    | 2.41                     | 0.53              |
| 33:BG:170:ARG:HH21 | 33:BG:182:LYS:NZ   | 2.06                     | 0.53              |
| 37:BO:102:VAL:HB   | 37:BO:106:LEU:HD12 | 1.90                     | 0.53              |
| 37:BO:13:ASN:CG    | 37:BO:97:ARG:HB2   | 2.29                     | 0.53              |
| 38:BP:61:ARG:HH11  | 57:B8:13:ARG:HD2   | 1.74                     | 0.53              |
| 27:BA:2483:C:H2'   | 39:BQ:49:ALA:HB1   | 1.90                     | 0.53              |
| 39:BQ:77:LYS:NZ    | 39:BQ:84:GLY:O     | 2.25                     | 0.53              |
| 41:BS:95:HIS:CG    | 41:BS:96:GLY:N     | 2.75                     | 0.53              |
| 42:BT:79:HIS:C     | 42:BT:81:PRO:HD3   | 2.27                     | 0.53              |
| 44:BV:40:LEU:H     | 44:BV:47:VAL:CG1   | 2.20                     | 0.53              |
| 47:BY:45:VAL:HG12  | 47:BY:46:LYS:H     | 1.73                     | 0.53              |
| 1:CA:1032:G:H2'    | 1:CA:1033:G:H8     | 1.71                     | 0.53              |
| 1:CA:1085:U:O2'    | 1:CA:1086:U:OP1    | 2.23                     | 0.53              |
| 1:CA:116:A:H2'     | 1:CA:117:G:H8      | 1.71                     | 0.53              |
| 1:CA:1269:A:H5'    | 21:CU:18:TYR:O     | 2.07                     | 0.53              |
| 1:CA:23:C:O2'      | 1:CA:24:U:H5'      | 2.08                     | 0.53              |
| 1:CA:287:U:O2'     | 1:CA:288:A:H5'     | 2.07                     | 0.53              |
| 1:CA:666:G:H2'     | 1:CA:667:G:H8      | 1.72                     | 0.53              |
| 1:CA:818:G:C2'     | 1:CA:819:A:H5''    | 2.38                     | 0.53              |
| 3:CC:190:ARG:HG2   | 3:CC:190:ARG:NH1   | 2.24                     | 0.53              |
| 4:CD:30:LYS:C      | 4:CD:32:ALA:N      | 2.54                     | 0.53              |
| 5:CE:28:PHE:O      | 5:CE:47:LYS:HA     | 2.08                     | 0.53              |
| 9:CI:79:LEU:HD13   | 9:CI:79:LEU:O      | 2.08                     | 0.53              |
| 10:CJ:30:SER:HB3   | 10:CJ:80:LYS:CE    | 2.39                     | 0.53              |
| 12:CL:43:LYS:NZ    | 12:CL:44:LYS:HE2   | 2.23                     | 0.53              |
| 1:CA:1228:C:H4'    | 13:CM:116:THR:HA   | 1.90                     | 0.53              |
| 14:CN:24:CYS:HB2   | 14:CN:40:CYS:HB3   | 1.88                     | 0.53              |
| 1:CA:742:G:H5'     | 15:CO:58:MET:HE1   | 1.87                     | 0.53              |
| 19:CS:32:LYS:HG3   | 19:CS:50:ALA:HB3   | 1.88                     | 0.53              |
| 51:D2:13:ALA:O     | 51:D2:15:LYS:N     | 2.40                     | 0.53              |
| 27:DA:1377:G:H8    | 27:DA:1377:G:O5'   | 1.91                     | 0.53              |
| 27:DA:49:A:N6      | 27:DA:177:G:H2'    | 2.12                     | 0.53              |
| 27:DA:2231:C:O2'   | 27:DA:2232:U:H5'   | 2.09                     | 0.53              |
| 27:DA:2290:G:C8    | 27:DA:2290:G:H5'   | 2.35                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:2340:G:H2'  | 27:DA:2341:G:C8    | 2.42                     | 0.53              |
| 27:DA:2550:G:O2'  | 27:DA:2551:C:H5'   | 2.08                     | 0.53              |
| 27:DA:298:G:OP1   | 47:DY:85:VAL:HG23  | 2.08                     | 0.53              |
| 28:DB:71:C:H2'    | 28:DB:72:G:H5'     | 1.90                     | 0.53              |
| 29:DC:49:ILE:HD12 | 29:DC:49:ILE:N     | 2.20                     | 0.53              |
| 30:DD:67:PHE:HB3  | 30:DD:153:ALA:HB3  | 1.89                     | 0.53              |
| 27:DA:2513:G:N2   | 31:DE:143:ASN:HD21 | 2.06                     | 0.53              |
| 31:DE:51:PHE:HE1  | 31:DE:52:LEU:HD13  | 1.70                     | 0.53              |
| 32:DF:139:PHE:HB2 | 32:DF:166:ALA:HB1  | 1.90                     | 0.53              |
| 34:DH:94:TYR:CG   | 34:DH:107:VAL:HG12 | 2.42                     | 0.53              |
| 40:DR:16:HIS:C    | 40:DR:18:LEU:N     | 2.59                     | 0.53              |
| 44:DV:5:VAL:HG21  | 44:DV:35:LEU:HG    | 1.90                     | 0.53              |
| 47:DY:2:ARG:O     | 47:DY:3:VAL:CB     | 2.56                     | 0.53              |
| 1:AA:1445:C:O2'   | 1:AA:1446:U:H5'    | 2.09                     | 0.53              |
| 1:AA:492:G:C4     | 1:AA:493:G:C8      | 2.97                     | 0.53              |
| 1:AA:567:G:N2     | 1:AA:568:G:H1'     | 2.23                     | 0.53              |
| 1:AA:670:G:O2'    | 1:AA:671:G:H5'     | 2.09                     | 0.53              |
| 1:AA:706:A:H1'    | 11:AK:29:ILE:HD11  | 1.89                     | 0.53              |
| 4:AD:154:ASN:O    | 4:AD:155:LEU:HD23  | 2.08                     | 0.53              |
| 10:AJ:29:ARG:HH22 | 10:AJ:84:GLN:HG2   | 1.73                     | 0.53              |
| 14:AN:24:CYS:HB2  | 14:AN:40:CYS:HB3   | 1.90                     | 0.53              |
| 15:AO:37:ASN:H    | 15:AO:37:ASN:ND2   | 2.00                     | 0.53              |
| 16:AP:58:TYR:O    | 16:AP:61:SER:OG    | 2.22                     | 0.53              |
| 16:AP:74:LEU:HB3  | 16:AP:79:VAL:CG2   | 2.38                     | 0.53              |
| 19:AS:48:THR:HG22 | 19:AS:61:TYR:HA    | 1.89                     | 0.53              |
| 23:AW:22:G:C2'    | 23:AW:23:G:H5'     | 2.36                     | 0.53              |
| 23:AW:23:G:H2'    | 23:AW:24:C:C6      | 2.44                     | 0.53              |
| 24:AX:64:G:H2'    | 24:AX:65:C:H6      | 1.74                     | 0.53              |
| 49:B0:51:VAL:HG23 | 49:B0:81:VAL:HG23  | 1.90                     | 0.53              |
| 51:B2:31:GLU:O    | 51:B2:35:LEU:HB2   | 2.08                     | 0.53              |
| 51:B2:42:GLY:C    | 51:B2:44:LEU:N     | 2.62                     | 0.53              |
| 27:BA:685:A:OP1   | 56:B7:11:LYS:NZ    | 2.41                     | 0.53              |
| 27:BA:1683:C:H2'  | 27:BA:1684:C:H6    | 1.73                     | 0.53              |
| 27:BA:1957:C:H2'  | 27:BA:1958:C:C6    | 2.44                     | 0.53              |
| 27:BA:231:C:H2'   | 27:BA:232:G:O4'    | 2.07                     | 0.53              |
| 27:BA:2555:U:H2'  | 27:BA:2556:C:C5'   | 2.38                     | 0.53              |
| 27:BA:2555:U:H2'  | 27:BA:2556:C:H5'   | 1.90                     | 0.53              |
| 27:BA:2683:C:OP1  | 42:BT:53:ARG:NH2   | 2.41                     | 0.53              |
| 27:BA:638:G:C5    | 27:BA:639:U:C4     | 2.97                     | 0.53              |
| 27:BA:802:A:C5    | 27:BA:803:U:C4     | 2.96                     | 0.53              |
| 29:BC:99:ILE:HG22 | 29:BC:99:ILE:O     | 2.08                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BD:79:VAL:CG1  | 30:BD:79:VAL:O     | 2.57                     | 0.53              |
| 32:BF:47:GLY:O    | 32:BF:94:PRO:HA    | 2.08                     | 0.53              |
| 37:BO:66:LYS:O    | 37:BO:78:ARG:HD3   | 2.08                     | 0.53              |
| 38:BP:106:LEU:O   | 38:BP:107:LYS:HG2  | 2.08                     | 0.53              |
| 38:BP:120:ALA:HB1 | 38:BP:138:LEU:HD13 | 1.89                     | 0.53              |
| 38:BP:34:GLY:O    | 38:BP:35:HIS:HB2   | 2.08                     | 0.53              |
| 39:BQ:58:PHE:O    | 39:BQ:59:ARG:C     | 2.47                     | 0.53              |
| 43:BU:95:LEU:HD22 | 44:BV:4:ILE:HD13   | 1.88                     | 0.53              |
| 47:BY:76:CYS:O    | 47:BY:77:PRO:C     | 2.47                     | 0.53              |
| 48:BZ:38:VAL:CG2  | 48:BZ:43:PHE:HB2   | 2.37                     | 0.53              |
| 48:BZ:52:ILE:H    | 48:BZ:52:ILE:HD12  | 1.72                     | 0.53              |
| 1:CA:1119:C:H2'   | 1:CA:1120:G:C8     | 2.42                     | 0.53              |
| 1:CA:122:G:O2'    | 1:CA:123:C:H5'     | 2.09                     | 0.53              |
| 1:CA:1301:U:H2'   | 1:CA:1303:C:H5     | 1.72                     | 0.53              |
| 1:CA:370:C:O2'    | 1:CA:371:G:H5'     | 2.08                     | 0.53              |
| 1:CA:815:A:H2'    | 1:CA:1526:G:H21    | 1.72                     | 0.53              |
| 1:CA:818:G:C3'    | 1:CA:819:A:H5''    | 2.38                     | 0.53              |
| 2:CB:223:ILE:HA   | 2:CB:226:ARG:HB3   | 1.90                     | 0.53              |
| 5:CE:97:GLY:N     | 5:CE:117:ASP:OD1   | 2.41                     | 0.53              |
| 6:CF:33:TYR:CE2   | 6:CF:74:ASP:HB3    | 2.43                     | 0.53              |
| 11:CK:34:ASP:HB2  | 11:CK:35:PRO:CD    | 2.38                     | 0.53              |
| 11:CK:15:ALA:HB1  | 11:CK:78:GLN:CG    | 2.38                     | 0.53              |
| 13:CM:29:ARG:HB3  | 13:CM:64:TRP:CZ2   | 2.43                     | 0.53              |
| 13:CM:23:TYR:HD1  | 13:CM:67:GLU:HA    | 1.73                     | 0.53              |
| 17:CQ:4:LYS:HG3   | 17:CQ:6:LEU:CD1    | 2.39                     | 0.53              |
| 19:CS:6:LYS:H     | 19:CS:6:LYS:CE     | 2.21                     | 0.53              |
| 24:CX:10:G:H22    | 24:CX:26:G:H1'     | 1.70                     | 0.53              |
| 38:DP:65:ARG:NH2  | 57:D8:15:LYS:HB2   | 2.23                     | 0.53              |
| 27:DA:1146:C:C2'  | 27:DA:1147:C:H5'   | 2.38                     | 0.53              |
| 27:DA:176:G:H2'   | 27:DA:177:G:O4'    | 2.08                     | 0.53              |
| 27:DA:204:A:O2'   | 27:DA:205:G:H4'    | 2.07                     | 0.53              |
| 27:DA:2139:C:H2'  | 27:DA:2140:C:H6    | 1.73                     | 0.53              |
| 27:DA:474:G:O2'   | 27:DA:475:U:OP1    | 2.24                     | 0.53              |
| 27:DA:638:G:H2'   | 27:DA:639:U:C6     | 2.43                     | 0.53              |
| 27:DA:966:G:H2'   | 27:DA:967:C:C6     | 2.43                     | 0.53              |
| 28:DB:12:C:O2'    | 28:DB:13:A:P       | 2.66                     | 0.53              |
| 30:DD:31:LYS:O    | 30:DD:32:SER:C     | 2.46                     | 0.53              |
| 31:DE:14:ILE:O    | 31:DE:21:VAL:HG22  | 2.08                     | 0.53              |
| 33:DG:91:ARG:C    | 33:DG:91:ARG:HD2   | 2.28                     | 0.53              |
| 42:DT:93:ARG:HG3  | 42:DT:93:ARG:NH1   | 2.21                     | 0.53              |
| 48:DZ:97:MET:H    | 48:DZ:124:LEU:HD12 | 1.72                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1026:G:H3'   | 1:AA:1027:C:C5'   | 2.39                     | 0.53              |
| 1:AA:1029:C:H4'   | 1:AA:1033:G:H1    | 1.73                     | 0.53              |
| 1:AA:1285:A:O4'   | 1:AA:1286:A:H8    | 1.92                     | 0.53              |
| 1:AA:1525:G:H2'   | 1:AA:1526:G:H8    | 1.72                     | 0.53              |
| 1:AA:159:G:N2     | 1:AA:162:A:OP2    | 2.41                     | 0.53              |
| 1:AA:936:C:O2'    | 1:AA:937:A:H5'    | 2.09                     | 0.53              |
| 3:AC:20:SER:HB2   | 3:AC:40:ARG:HH22  | 1.73                     | 0.53              |
| 3:AC:42:LEU:HD23  | 3:AC:46:GLU:OE2   | 2.08                     | 0.53              |
| 4:AD:188:LEU:CD2  | 4:AD:189:PRO:HD2  | 2.37                     | 0.53              |
| 6:AF:16:GLN:CD    | 6:AF:16:GLN:N     | 2.61                     | 0.53              |
| 6:AF:69:GLU:OE1   | 6:AF:69:GLU:N     | 2.37                     | 0.53              |
| 9:AI:92:TYR:O     | 9:AI:95:LYS:HG3   | 2.09                     | 0.53              |
| 11:AK:38:ASN:ND2  | 11:AK:38:ASN:N    | 2.54                     | 0.53              |
| 18:AR:59:SER:O    | 18:AR:60:ALA:C    | 2.45                     | 0.53              |
| 1:AA:1318:A:O3'   | 19:AS:10:PHE:CD2  | 2.61                     | 0.53              |
| 20:AT:98:PRO:O    | 20:AT:100:ILE:N   | 2.42                     | 0.53              |
| 49:B0:46:LYS:HB3  | 49:B0:47:PRO:HD2  | 1.90                     | 0.53              |
| 50:B1:50:ARG:HH11 | 50:B1:50:ARG:HG2  | 1.73                     | 0.53              |
| 55:B6:13:CYS:HB2  | 55:B6:22:ALA:HB3  | 1.90                     | 0.53              |
| 57:B8:47:LYS:HD2  | 57:B8:48:PHE:O    | 2.09                     | 0.53              |
| 27:BA:1011:G:OP1  | 43:BU:77:SER:HB3  | 2.08                     | 0.53              |
| 27:BA:1179:C:O2'  | 27:BA:1180:C:H5'' | 2.07                     | 0.53              |
| 27:BA:1223:G:N2   | 27:BA:1226:A:OP2  | 2.38                     | 0.53              |
| 27:BA:1268:A:H2'  | 27:BA:1269:A:C5'  | 2.38                     | 0.53              |
| 27:BA:1722:A:N6   | 27:BA:1741:A:N1   | 2.56                     | 0.53              |
| 27:BA:2001:A:H2'  | 27:BA:2002:G:C8   | 2.43                     | 0.53              |
| 27:BA:210:C:O2'   | 27:BA:211:A:H5'   | 2.09                     | 0.53              |
| 27:BA:2225:A:H4'  | 27:BA:2226:C:C6   | 2.43                     | 0.53              |
| 27:BA:2484:G:O2'  | 27:BA:2485:G:H5'  | 2.09                     | 0.53              |
| 27:BA:363(A):A:C4 | 27:BA:363(B):G:C8 | 2.96                     | 0.53              |
| 27:BA:543:C:O3'   | 27:BA:547:A:P     | 2.66                     | 0.53              |
| 27:BA:559:G:N2    | 43:BU:49:HIS:CD2  | 2.76                     | 0.53              |
| 27:BA:577:G:H8    | 27:BA:577:G:O5'   | 1.91                     | 0.53              |
| 27:BA:686:G:O6    | 56:B7:12:ARG:HG3  | 2.07                     | 0.53              |
| 27:BA:953:A:OP2   | 39:BQ:16:ARG:NH2  | 2.41                     | 0.53              |
| 28:BB:94:C:H2'    | 28:BB:95:C:C6     | 2.44                     | 0.53              |
| 30:BD:35:LYS:HZ3  | 30:BD:103:ARG:N   | 2.06                     | 0.53              |
| 27:BA:2227:A:H5'  | 30:BD:263:ARG:NH1 | 2.23                     | 0.53              |
| 30:BD:30:GLU:CD   | 30:BD:63:ARG:HH21 | 2.12                     | 0.53              |
| 34:BH:169:VAL:O   | 34:BH:171:LEU:N   | 2.41                     | 0.53              |
| 27:BA:2880:C:H1'  | 40:BR:92:GLY:O    | 2.07                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BT:102:ILE:HG22 | 42:BT:110:ILE:HG12 | 1.89                     | 0.53              |
| 43:BU:61:TRP:CE2   | 43:BU:94:ASN:HA    | 2.43                     | 0.53              |
| 46:BX:18:TYR:C     | 46:BX:20:GLY:H     | 2.11                     | 0.53              |
| 1:CA:68:G:C6       | 1:CA:102:G:N1      | 2.76                     | 0.53              |
| 1:CA:1106:G:H4'    | 3:CC:171:GLY:O     | 2.08                     | 0.53              |
| 1:CA:1117:G:O2'    | 9:CI:104:ARG:HG3   | 2.08                     | 0.53              |
| 1:CA:1290:G:N3     | 1:CA:1290:G:H2'    | 2.22                     | 0.53              |
| 1:CA:444:C:H2'     | 1:CA:445:G:H8      | 1.72                     | 0.53              |
| 1:CA:658:G:C2      | 1:CA:659:U:C2      | 2.96                     | 0.53              |
| 1:CA:939:G:C6      | 1:CA:940:C:N4      | 2.76                     | 0.53              |
| 2:CB:124:SER:O     | 2:CB:126:GLU:N     | 2.41                     | 0.53              |
| 2:CB:147:LYS:HE2   | 2:CB:148:TYR:HE1   | 1.71                     | 0.53              |
| 3:CC:135:LYS:HZ1   | 5:CE:53:LEU:HD21   | 1.74                     | 0.53              |
| 3:CC:184:TYR:HA    | 3:CC:200:ALA:O     | 2.08                     | 0.53              |
| 3:CC:83:ARG:HG2    | 3:CC:83:ARG:HH11   | 1.73                     | 0.53              |
| 6:CF:30:LEU:HA     | 6:CF:75:LEU:HD11   | 1.90                     | 0.53              |
| 8:CH:6:ILE:CG2     | 8:CH:10:LEU:HD12   | 2.38                     | 0.53              |
| 8:CH:80:ILE:HG22   | 8:CH:82:HIS:O      | 2.09                     | 0.53              |
| 25:CY:42:G:C2'     | 25:CY:43:C:H5'     | 2.38                     | 0.53              |
| 50:D1:7:ILE:HG22   | 50:D1:8:SER:N      | 2.22                     | 0.53              |
| 55:D6:12:GLU:HB2   | 55:D6:21:TYR:HB3   | 1.91                     | 0.53              |
| 56:D7:19:ARG:HH11  | 56:D7:19:ARG:HG3   | 1.73                     | 0.53              |
| 27:DA:1164:G:H1    | 27:DA:1185:C:N4    | 2.04                     | 0.53              |
| 27:DA:2391:G:N1    | 27:DA:2424:C:H2'   | 2.23                     | 0.53              |
| 27:DA:2476:A:H2'   | 27:DA:2477:C:C5'   | 2.37                     | 0.53              |
| 27:DA:2694:G:O2'   | 27:DA:2695:C:H5'   | 2.08                     | 0.53              |
| 27:DA:2712:U:H1'   | 27:DA:2712(A):A:C8 | 2.44                     | 0.53              |
| 27:DA:2772:C:H2'   | 27:DA:2773:C:C6    | 2.43                     | 0.53              |
| 27:DA:2855:C:H2'   | 27:DA:2856:C:H6    | 1.73                     | 0.53              |
| 27:DA:477:A:C2     | 27:DA:478:A:C4     | 2.97                     | 0.53              |
| 27:DA:587:C:O2'    | 27:DA:588:U:OP2    | 2.21                     | 0.53              |
| 28:DB:20:C:H2'     | 28:DB:21:G:H5'     | 1.87                     | 0.53              |
| 29:DC:59:ARG:N     | 29:DC:59:ARG:HD3   | 2.23                     | 0.53              |
| 30:DD:231:HIS:CG   | 30:DD:232:PRO:HD2  | 2.40                     | 0.53              |
| 31:DE:36:ARG:HH22  | 31:DE:88:GLY:N     | 2.05                     | 0.53              |
| 35:DI:133:HIS:CG   | 35:DI:134:PRO:HD3  | 2.44                     | 0.53              |
| 27:DA:245:G:H5'    | 38:DP:69:GLY:HA3   | 1.90                     | 0.53              |
| 39:DQ:76:LYS:HA    | 39:DQ:76:LYS:HE2   | 1.90                     | 0.53              |
| 41:DS:59:LYS:HE3   | 41:DS:68:GLN:NE2   | 2.23                     | 0.53              |
| 42:DT:48:ILE:HG22  | 42:DT:50:ILE:CD1   | 2.39                     | 0.53              |
| 44:DV:19:LYS:HG3   | 44:DV:20:LEU:O     | 2.08                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:DW:7:ALA:O     | 45:DW:103:ILE:N    | 2.31                     | 0.53              |
| 47:DY:7:VAL:HG21  | 47:DY:8:LYS:NZ     | 2.22                     | 0.53              |
| 48:DZ:150:HIS:CB  | 48:DZ:169:THR:HA   | 2.38                     | 0.53              |
| 1:AA:103:C:C4     | 1:AA:104:G:N7      | 2.76                     | 0.53              |
| 1:AA:1211:U:H4'   | 1:AA:1212:U:OP1    | 2.08                     | 0.53              |
| 1:AA:1311:G:H1    | 1:AA:1326:C:H42    | 1.56                     | 0.53              |
| 1:AA:1498:U:C4    | 22:AV:5:U:H4'      | 2.44                     | 0.53              |
| 1:AA:1517:G:H2'   | 1:AA:1518:A:H8     | 1.70                     | 0.53              |
| 1:AA:660:G:H2'    | 1:AA:661:G:H8      | 1.72                     | 0.53              |
| 1:AA:953:G:C5'    | 1:AA:965:A:H61     | 2.21                     | 0.53              |
| 2:AB:155:LEU:HG   | 2:AB:159:PRO:HG3   | 1.89                     | 0.53              |
| 4:AD:94:LEU:HD23  | 4:AD:97:LEU:HD12   | 1.90                     | 0.53              |
| 7:AG:30:ILE:HB    | 7:AG:39:ALA:HB1    | 1.89                     | 0.53              |
| 8:AH:4:ASP:CG     | 8:AH:85:ARG:HH12   | 2.12                     | 0.53              |
| 11:AK:80:VAL:HG13 | 11:AK:103:LEU:HD11 | 1.90                     | 0.53              |
| 13:AM:76:ALA:HB2  | 13:AM:79:LYS:HZ3   | 1.72                     | 0.53              |
| 20:AT:93:GLU:O    | 20:AT:93:GLU:HG2   | 2.08                     | 0.53              |
| 23:AW:4:G:C3'     | 23:AW:5:G:H5''     | 2.38                     | 0.53              |
| 49:B0:69:PHE:CD1  | 49:B0:69:PHE:N     | 2.76                     | 0.53              |
| 54:B5:33:CYS:O    | 54:B5:36:CYS:O     | 2.24                     | 0.53              |
| 27:BA:1786:A:N1   | 27:BA:2606:C:O4'   | 2.41                     | 0.53              |
| 27:BA:184:C:H2'   | 27:BA:185:U:C6     | 2.42                     | 0.53              |
| 27:BA:1925:C:C2'  | 27:BA:1926:U:O5'   | 2.56                     | 0.53              |
| 27:BA:207:A:H2'   | 27:BA:208:C:O4'    | 2.07                     | 0.53              |
| 27:BA:221:A:O2'   | 27:BA:222:A:OP2    | 2.20                     | 0.53              |
| 27:BA:257:A:C5    | 27:BA:258:G:C8     | 2.97                     | 0.53              |
| 27:BA:385:C:O2    | 27:BA:390:A:H2     | 1.91                     | 0.53              |
| 27:BA:556:G:H2'   | 27:BA:557:U:H6     | 1.72                     | 0.53              |
| 27:BA:626:U:C5'   | 27:BA:627:A:C5'    | 2.85                     | 0.53              |
| 27:BA:790:C:O2'   | 27:BA:791:C:H5'    | 2.08                     | 0.53              |
| 31:BE:28:ALA:HB3  | 31:BE:93:VAL:HG22  | 1.89                     | 0.53              |
| 32:BF:2:LYS:O     | 32:BF:25:PRO:HD2   | 2.08                     | 0.53              |
| 34:BH:85:LYS:HZ2  | 34:BH:133:VAL:HG21 | 1.71                     | 0.53              |
| 38:BP:16:ARG:CD   | 38:BP:18:ARG:H     | 2.18                     | 0.53              |
| 41:BS:12:PHE:CD1  | 41:BS:12:PHE:O     | 2.61                     | 0.53              |
| 42:BT:89:VAL:CG1  | 42:BT:91:ARG:HE    | 2.20                     | 0.53              |
| 47:BY:20:TYR:HD2  | 47:BY:23:ARG:HD3   | 1.72                     | 0.53              |
| 1:CA:505:G:C6     | 1:CA:535:A:C2      | 2.97                     | 0.53              |
| 3:CC:101:LEU:HD23 | 3:CC:102:ASN:N     | 2.22                     | 0.53              |
| 3:CC:63:ASN:HA    | 3:CC:98:ASN:HB3    | 1.90                     | 0.53              |
| 4:CD:190:ASP:N    | 4:CD:193:ASP:OD2   | 2.41                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CD:36:ARG:C     | 4:CD:38:TYR:H      | 2.11                     | 0.53              |
| 13:CM:89:GLY:C    | 13:CM:93:ARG:HD2   | 2.28                     | 0.53              |
| 49:D0:10:THR:HG22 | 49:D0:12:ASN:H     | 1.74                     | 0.53              |
| 27:DA:750:A:OP1   | 27:DA:1615:C:N4    | 2.41                     | 0.53              |
| 27:DA:2011:U:C2'  | 27:DA:2012:G:H5'   | 2.39                     | 0.53              |
| 27:DA:2489:G:N7   | 27:DA:2490:G:C6    | 2.77                     | 0.53              |
| 27:DA:2056:G:N7   | 27:DA:2577:A:N7    | 2.55                     | 0.53              |
| 27:DA:454:A:O2'   | 27:DA:455:C:OP1    | 2.24                     | 0.53              |
| 27:DA:534:U:H5'   | 43:DU:42:ALA:HB1   | 1.89                     | 0.53              |
| 27:DA:555:U:H2'   | 27:DA:556:G:C8     | 2.43                     | 0.53              |
| 27:DA:779:U:P     | 30:DD:49:ILE:HG22  | 2.49                     | 0.53              |
| 27:DA:802:A:H2'   | 27:DA:803:U:C6     | 2.44                     | 0.53              |
| 27:DA:950:G:C6    | 27:DA:968:G:C6     | 2.96                     | 0.53              |
| 28:DB:24:G:H1'    | 28:DB:27:C:H41     | 1.72                     | 0.53              |
| 29:DC:59:ARG:NH2  | 29:DC:197:GLU:O    | 2.37                     | 0.53              |
| 30:DD:62:TYR:HA   | 30:DD:87:ASN:ND2   | 2.23                     | 0.53              |
| 31:DE:34:VAL:O    | 31:DE:35:GLN:CB    | 2.55                     | 0.53              |
| 35:DI:75:LEU:HD12 | 35:DI:76:THR:H     | 1.73                     | 0.53              |
| 36:DN:67:LEU:HB3  | 36:DN:88:GLU:OE2   | 2.09                     | 0.53              |
| 37:DO:10:VAL:HG13 | 37:DO:17:ARG:O     | 2.08                     | 0.53              |
| 37:DO:66:LYS:CD   | 37:DO:79:PHE:O     | 2.54                     | 0.53              |
| 37:DO:86:ILE:HG21 | 37:DO:94:ARG:HD2   | 1.90                     | 0.53              |
| 38:DP:97:PRO:HD3  | 38:DP:126:VAL:HB   | 1.90                     | 0.53              |
| 38:DP:97:PRO:C    | 38:DP:99:LEU:H     | 2.11                     | 0.53              |
| 38:DP:97:PRO:O    | 38:DP:98:GLU:HB3   | 2.08                     | 0.53              |
| 39:DQ:38:GLU:O    | 39:DQ:127:ILE:HG21 | 2.07                     | 0.53              |
| 39:DQ:73:PRO:HG3  | 39:DQ:93:TYR:HE2   | 1.74                     | 0.53              |
| 40:DR:81:ASP:N    | 40:DR:81:ASP:OD2   | 2.41                     | 0.53              |
| 41:DS:89:ARG:HD2  | 41:DS:92:TYR:CA    | 2.37                     | 0.53              |
| 42:DT:80:SER:CB   | 42:DT:81:PRO:CD    | 2.86                     | 0.53              |
| 43:DU:78:THR:O    | 43:DU:79:PHE:C     | 2.46                     | 0.53              |
| 47:DY:100:ALA:O   | 47:DY:101:LYS:O    | 2.26                     | 0.53              |
| 48:DZ:165:SER:H   | 48:DZ:166:PRO:HA   | 1.73                     | 0.53              |
| 1:AA:1060:C:H2'   | 1:AA:1061:G:C8     | 2.42                     | 0.53              |
| 1:AA:185:A:H2'    | 1:AA:186:C:C6      | 2.43                     | 0.53              |
| 1:AA:502:G:O2'    | 1:AA:503:C:H5'     | 2.09                     | 0.53              |
| 1:AA:858:G:O6     | 1:AA:869:G:C8      | 2.62                     | 0.53              |
| 8:AH:109:ILE:HD11 | 8:AH:120:THR:HG22  | 1.91                     | 0.53              |
| 8:AH:4:ASP:OD2    | 8:AH:6:ILE:HD13    | 2.08                     | 0.53              |
| 8:AH:74:PRO:O     | 8:AH:75:ARG:C      | 2.46                     | 0.53              |
| 10:AJ:34:VAL:HG13 | 10:AJ:73:ASP:C     | 2.29                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:AM:111:LYS:O   | 13:AM:112:GLY:O    | 2.25                     | 0.53              |
| 20:AT:89:ARG:HH21 | 20:AT:104:LEU:HD11 | 1.73                     | 0.53              |
| 50:B1:70:VAL:C    | 50:B1:72:GLU:H     | 2.12                     | 0.53              |
| 51:B2:6:VAL:HG13  | 51:B2:59:ARG:NH1   | 2.24                     | 0.53              |
| 55:B6:16:CYS:SG   | 55:B6:48:VAL:HG23  | 2.49                     | 0.53              |
| 58:B9:12:ASP:OD1  | 58:B9:13:LYS:N     | 2.41                     | 0.53              |
| 27:BA:114:U:N3    | 27:BA:115:C:C4     | 2.76                     | 0.53              |
| 27:BA:1466:G:H5'  | 27:BA:1467:C:OP1   | 2.08                     | 0.53              |
| 27:BA:1491:G:P    | 27:BA:1494:A:H62   | 2.30                     | 0.53              |
| 27:BA:1655:A:H3'  | 27:BA:1656:C:C6    | 2.44                     | 0.53              |
| 27:BA:1790:C:H2'  | 27:BA:1791:A:C5    | 2.43                     | 0.53              |
| 27:BA:2183:C:O2'  | 27:BA:2184:G:H5'   | 2.08                     | 0.53              |
| 27:BA:855:G:H2'   | 27:BA:856:C:H6     | 1.74                     | 0.53              |
| 29:BC:38:ASP:HB2  | 29:BC:181:PRO:CB   | 2.38                     | 0.53              |
| 30:BD:65:ILE:HB   | 30:BD:104:TYR:HB3  | 1.90                     | 0.53              |
| 32:BF:37:VAL:HG13 | 32:BF:184:TYR:HD1  | 1.74                     | 0.53              |
| 32:BF:29:ASN:HB3  | 32:BF:112:MET:CE   | 2.34                     | 0.53              |
| 33:BG:96:ARG:O    | 33:BG:99:MET:N     | 2.29                     | 0.53              |
| 36:BN:22:THR:HA   | 36:BN:61:ARG:HB2   | 1.89                     | 0.53              |
| 38:BP:124:LYS:HE3 | 38:BP:145:PRO:HG2  | 1.89                     | 0.53              |
| 39:BQ:34:LEU:HD12 | 39:BQ:130:LYS:O    | 2.07                     | 0.53              |
| 42:BT:30:VAL:HG21 | 42:BT:83:ILE:CG1   | 2.38                     | 0.53              |
| 44:BV:35:LEU:CA   | 44:BV:37:VAL:HG23  | 2.38                     | 0.53              |
| 46:BX:26:TYR:HB3  | 46:BX:92:LEU:CD1   | 2.39                     | 0.53              |
| 48:BZ:149:LEU:N   | 48:BZ:149:LEU:HD13 | 2.23                     | 0.53              |
| 1:CA:1055:A:N6    | 1:CA:1206:G:C6     | 2.77                     | 0.53              |
| 1:CA:178:C:H2'    | 1:CA:179:A:C8      | 2.43                     | 0.53              |
| 1:CA:274:A:O2'    | 1:CA:275:G:O5'     | 2.26                     | 0.53              |
| 1:CA:885:G:C2     | 1:CA:913:A:C2      | 2.97                     | 0.53              |
| 1:CA:971:G:O2'    | 1:CA:1365:G:O2'    | 2.24                     | 0.53              |
| 2:CB:219:VAL:HA   | 2:CB:222:ILE:CD1   | 2.38                     | 0.53              |
| 3:CC:97:LYS:O     | 3:CC:99:VAL:N      | 2.37                     | 0.53              |
| 10:CJ:16:LEU:HD11 | 10:CJ:70:ARG:HB2   | 1.91                     | 0.53              |
| 11:CK:98:LEU:HA   | 11:CK:101:SER:HB3  | 1.89                     | 0.53              |
| 12:CL:22:PRO:C    | 12:CL:24:LEU:N     | 2.62                     | 0.53              |
| 13:CM:29:ARG:HD3  | 13:CM:64:TRP:CH2   | 2.44                     | 0.53              |
| 16:CP:45:THR:O    | 16:CP:47:ASP:N     | 2.41                     | 0.53              |
| 20:CT:16:HIS:CA   | 20:CT:19:SER:HB3   | 2.37                     | 0.53              |
| 1:CA:1459:C:H5'   | 20:CT:28:ALA:HB2   | 1.91                     | 0.53              |
| 20:CT:96:GLY:O    | 20:CT:97:ALA:O     | 2.27                     | 0.53              |
| 24:CX:17:C:C2     | 24:CX:17(B):U:H5   | 2.27                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CX:47:U:H3'     | 24:CX:48:C:H5'     | 1.91                     | 0.53              |
| 50:D1:29:GLY:O     | 50:D1:30:VAL:HG23  | 2.08                     | 0.53              |
| 52:D3:44:ARG:O     | 52:D3:48:GLU:HG2   | 2.08                     | 0.53              |
| 55:D6:9:LEU:HD21   | 55:D6:11:LEU:HD23  | 1.90                     | 0.53              |
| 27:DA:2420:C:P     | 57:D8:33:ASN:O     | 2.66                     | 0.53              |
| 27:DA:1173:G:H3'   | 27:DA:1174:A:C5'   | 2.39                     | 0.53              |
| 27:DA:1304:C:N4    | 27:DA:1624:G:H1    | 2.05                     | 0.53              |
| 27:DA:2293:C:H2'   | 27:DA:2294:C:H6    | 1.72                     | 0.53              |
| 27:DA:2714:G:H2'   | 27:DA:2715:C:H6    | 1.72                     | 0.53              |
| 27:DA:271(T):C:O2' | 27:DA:271(U):G:H5' | 2.07                     | 0.53              |
| 27:DA:2746:U:H2'   | 27:DA:2747:G:H5'   | 1.90                     | 0.53              |
| 27:DA:398:G:O2'    | 27:DA:399:G:H5'    | 2.09                     | 0.53              |
| 27:DA:696:G:C2     | 27:DA:697:C:C2     | 2.96                     | 0.53              |
| 27:DA:898:C:H2'    | 27:DA:899:A:C5'    | 2.37                     | 0.53              |
| 30:DD:71:ASP:HB2   | 30:DD:103:ARG:HH22 | 1.72                     | 0.53              |
| 30:DD:120:GLY:HA2  | 30:DD:190:TYR:OH   | 2.08                     | 0.53              |
| 31:DE:119:ARG:CD   | 31:DE:120:TRP:CD1  | 2.92                     | 0.53              |
| 32:DF:33:LEU:O     | 32:DF:37:VAL:HG23  | 2.09                     | 0.53              |
| 33:DG:130:ASN:OD1  | 33:DG:160:VAL:CG1  | 2.56                     | 0.53              |
| 38:DP:127:ALA:HB3  | 38:DP:130:PHE:CZ   | 2.43                     | 0.53              |
| 27:DA:1278:A:H5'   | 40:DR:24:GLN:HE21  | 1.73                     | 0.53              |
| 41:DS:53:SER:O     | 41:DS:58:LEU:HD22  | 2.07                     | 0.53              |
| 48:DZ:102:ARG:HB2  | 48:DZ:135:PHE:CE1  | 2.44                     | 0.53              |
| 48:DZ:66:LEU:HD23  | 48:DZ:89:VAL:HG11  | 1.90                     | 0.53              |
| 1:AA:1265:G:H2'    | 1:AA:1266:G:O4'    | 2.09                     | 0.53              |
| 1:AA:353:A:H5'     | 1:AA:353:A:H8      | 1.74                     | 0.53              |
| 1:AA:616:G:H2'     | 1:AA:616:G:N3      | 2.24                     | 0.53              |
| 2:AB:69:LEU:O      | 2:AB:162:ILE:HA    | 2.09                     | 0.53              |
| 2:AB:73:THR:O      | 2:AB:78:GLN:HG3    | 2.09                     | 0.53              |
| 3:AC:142:MET:HE2   | 3:AC:170:GLN:C     | 2.28                     | 0.53              |
| 7:AG:113:GLU:HG3   | 7:AG:119:ARG:HA    | 1.90                     | 0.53              |
| 8:AH:33:GLU:C      | 8:AH:35:ILE:H      | 2.12                     | 0.53              |
| 8:AH:4:ASP:OD1     | 8:AH:7:ALA:HB3     | 2.08                     | 0.53              |
| 10:AJ:8:LEU:CD2    | 10:AJ:96:ILE:HG22  | 2.39                     | 0.53              |
| 15:AO:3:ILE:HG22   | 15:AO:38:ARG:HH12  | 1.71                     | 0.53              |
| 16:AP:1:MET:SD     | 16:AP:1:MET:N      | 2.80                     | 0.53              |
| 17:AQ:60:ILE:HG12  | 17:AQ:61:GLU:N     | 2.22                     | 0.53              |
| 50:B1:77:ALA:O     | 50:B1:80:LEU:HB2   | 2.09                     | 0.53              |
| 27:BA:1274:A:H1'   | 27:BA:1297:C:C4'   | 2.39                     | 0.53              |
| 27:BA:2056:G:H2'   | 27:BA:2056:G:N3    | 2.24                     | 0.53              |
| 27:BA:2105:C:O2'   | 27:BA:2106:G:H5'   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2125:G:N2   | 27:BA:2174:C:H42   | 2.07                     | 0.53              |
| 27:BA:2272:U:H5'' | 27:BA:2273:A:OP1   | 2.09                     | 0.53              |
| 27:BA:2349:G:C4   | 27:BA:2369:A:C2    | 2.97                     | 0.53              |
| 27:BA:2723:C:OP1  | 40:BR:5:LYS:NZ     | 2.40                     | 0.53              |
| 27:BA:284:U:H2'   | 27:BA:285:C:C6     | 2.43                     | 0.53              |
| 27:BA:581:C:O5'   | 27:BA:581:C:H6     | 1.91                     | 0.53              |
| 27:BA:826:U:H5'   | 27:BA:827:U:OP2    | 2.07                     | 0.53              |
| 27:BA:849:A:C8    | 27:BA:850:C:C5     | 2.97                     | 0.53              |
| 31:BE:173:VAL:O   | 31:BE:174:ASP:C    | 2.47                     | 0.53              |
| 32:BF:184:TYR:O   | 32:BF:188:ARG:HB3  | 2.09                     | 0.53              |
| 32:BF:9:ILE:HB    | 32:BF:128:ALA:HB2  | 1.91                     | 0.53              |
| 35:BI:81:VAL:HB   | 35:BI:143:SER:O    | 2.08                     | 0.53              |
| 36:BN:96:GLU:N    | 36:BN:96:GLU:OE2   | 2.40                     | 0.53              |
| 37:BO:106:LEU:C   | 37:BO:108:GLU:H    | 2.12                     | 0.53              |
| 41:BS:17:ARG:O    | 41:BS:18:ILE:HG22  | 2.09                     | 0.53              |
| 42:BT:26:ASP:O    | 42:BT:26:ASP:OD2   | 2.27                     | 0.53              |
| 42:BT:46:GLU:OE2  | 42:BT:88:ILE:HD13  | 2.08                     | 0.53              |
| 45:BW:13:SER:HB3  | 45:BW:16:LYS:CG    | 2.39                     | 0.53              |
| 45:BW:13:SER:HB3  | 45:BW:16:LYS:HG3   | 1.90                     | 0.53              |
| 45:BW:62:HIS:O    | 45:BW:63:ASP:C     | 2.46                     | 0.53              |
| 45:BW:96:ILE:O    | 45:BW:96:ILE:HG23  | 2.09                     | 0.53              |
| 48:BZ:26:VAL:HG22 | 48:BZ:27:MET:N     | 2.23                     | 0.53              |
| 1:CA:1233:G:N2    | 1:CA:1234:C:C2     | 2.76                     | 0.53              |
| 1:CA:1313:U:H2'   | 1:CA:1314:C:H6     | 1.73                     | 0.53              |
| 1:CA:283:C:C2     | 1:CA:284:G:C8      | 2.97                     | 0.53              |
| 1:CA:360:A:O2'    | 1:CA:361:G:H5'     | 2.09                     | 0.53              |
| 1:CA:372:C:C5'    | 1:CA:373:A:OP1     | 2.57                     | 0.53              |
| 1:CA:376:G:OP2    | 16:CP:67:THR:HG21  | 2.08                     | 0.53              |
| 1:CA:778:G:O2'    | 1:CA:779:C:H5'     | 2.07                     | 0.53              |
| 12:CL:114:ARG:HG3 | 12:CL:114:ARG:HH11 | 1.72                     | 0.53              |
| 13:CM:35:GLU:HG3  | 13:CM:36:LYS:N     | 2.24                     | 0.53              |
| 15:CO:23:GLY:O    | 15:CO:24:SER:HB3   | 2.08                     | 0.53              |
| 17:CQ:67:LYS:O    | 17:CQ:68:ARG:CB    | 2.56                     | 0.53              |
| 21:CU:21:TYR:O    | 21:CU:22:ARG:CB    | 2.57                     | 0.53              |
| 55:D6:15:GLU:O    | 55:D6:15:GLU:HG2   | 2.09                     | 0.53              |
| 55:D6:15:GLU:OE1  | 55:D6:43:CYS:CB    | 2.56                     | 0.53              |
| 27:DA:1034:G:O2'  | 27:DA:1035:U:O5'   | 2.27                     | 0.53              |
| 27:DA:1152:C:H1'  | 43:DU:77:SER:HB2   | 1.91                     | 0.53              |
| 27:DA:1340:U:O2   | 27:DA:1603:A:H8    | 1.92                     | 0.53              |
| 27:DA:143:G:H5''  | 27:DA:1598:C:O2'   | 2.09                     | 0.53              |
| 27:DA:1621:U:H5'' | 27:DA:1622:G:OP1   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:1363:C:O2'  | 27:DA:1809:A:N3   | 2.27                     | 0.53              |
| 27:DA:2063:C:C5   | 27:DA:2064:C:C5   | 2.96                     | 0.53              |
| 27:DA:2143:C:H2'  | 27:DA:2144:U:O4'  | 2.09                     | 0.53              |
| 27:DA:2199:A:H5'  | 27:DA:2200:C:OP2  | 2.09                     | 0.53              |
| 27:DA:266:G:H2'   | 27:DA:267:C:O5'   | 2.09                     | 0.53              |
| 27:DA:356:G:H5'   | 27:DA:357:A:OP2   | 2.08                     | 0.53              |
| 27:DA:598:G:O2'   | 32:DF:31:HIS:CE1  | 2.61                     | 0.53              |
| 27:DA:875:G:H2'   | 27:DA:876:C:H6    | 1.74                     | 0.53              |
| 29:DC:45:ALA:HA   | 29:DC:210:ARG:CB  | 2.38                     | 0.53              |
| 31:DE:113:PHE:CD2 | 31:DE:113:PHE:C   | 2.80                     | 0.53              |
| 32:DF:32:LEU:HD22 | 32:DF:112:MET:CE  | 2.38                     | 0.53              |
| 35:DI:92:VAL:HG13 | 35:DI:120:ILE:HB  | 1.90                     | 0.53              |
| 35:DI:88:ILE:HG22 | 35:DI:90:GLY:O    | 2.08                     | 0.53              |
| 37:DO:87:ILE:HD13 | 37:DO:92:GLU:C    | 2.29                     | 0.53              |
| 39:DQ:20:ALA:O    | 39:DQ:99:PRO:HD2  | 2.08                     | 0.53              |
| 40:DR:13:HIS:O    | 40:DR:15:SER:N    | 2.42                     | 0.53              |
| 41:DS:67:ARG:CG   | 41:DS:67:ARG:HH11 | 2.20                     | 0.53              |
| 42:DT:32:TYR:HD1  | 42:DT:33:LYS:H    | 1.57                     | 0.53              |
| 44:DV:40:LEU:HD22 | 44:DV:40:LEU:N    | 2.24                     | 0.53              |
| 46:DX:57:LEU:HD22 | 46:DX:57:LEU:O    | 2.08                     | 0.53              |
| 47:DY:32:PRO:C    | 47:DY:35:TYR:H    | 2.10                     | 0.53              |
| 47:DY:8:LYS:C     | 47:DY:9:LYS:HG2   | 2.28                     | 0.53              |
| 1:AA:1182:G:O2'   | 1:AA:1183:A:OP2   | 2.24                     | 0.53              |
| 1:AA:144:G:H2'    | 1:AA:145:G:C8     | 2.44                     | 0.53              |
| 1:AA:256:U:O2'    | 1:AA:257:G:H5'    | 2.08                     | 0.53              |
| 1:AA:262:A:H5'    | 20:AT:74:LYS:CB   | 2.39                     | 0.53              |
| 1:AA:543:C:O2     | 1:AA:543:C:H2'    | 2.09                     | 0.53              |
| 1:AA:726:C:O2'    | 1:AA:727:G:H5'    | 2.08                     | 0.53              |
| 1:AA:937:A:H1'    | 1:AA:1379:G:N2    | 2.23                     | 0.53              |
| 5:AE:78:HIS:HD2   | 8:AH:104:ARG:NH1  | 2.07                     | 0.53              |
| 11:AK:126:ARG:C   | 11:AK:128:ALA:N   | 2.61                     | 0.53              |
| 51:B2:14:ARG:HH11 | 51:B2:14:ARG:HG3  | 1.74                     | 0.53              |
| 53:B4:41:ILE:H    | 53:B4:57:ILE:HG22 | 1.72                     | 0.53              |
| 27:BA:593:G:H1'   | 57:B8:4:MET:CE    | 2.39                     | 0.53              |
| 27:BA:1042:G:N3   | 27:BA:1042:G:H2'  | 2.23                     | 0.53              |
| 27:BA:1223:G:H5'  | 27:BA:1224:C:OP2  | 2.09                     | 0.53              |
| 27:BA:1931:U:C5'  | 27:BA:1931:U:H6   | 2.20                     | 0.53              |
| 27:BA:2134:A:H2   | 27:BA:2159:G:H1'  | 1.74                     | 0.53              |
| 27:BA:2299:G:C2   | 27:BA:2318:G:H8   | 2.26                     | 0.53              |
| 27:BA:2342:C:O2'  | 27:BA:2374:C:H5'' | 2.09                     | 0.53              |
| 30:BD:227:ASN:HB3 | 30:BD:228:PRO:HD2 | 1.90                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 32:BF:164:ARG:CG   | 32:BF:164:ARG:NH1   | 2.70                     | 0.53              |
| 32:BF:63:LYS:HZ2   | 32:BF:67:GLN:HB2    | 1.72                     | 0.53              |
| 33:BG:71:THR:N     | 33:BG:89:GLY:O      | 2.42                     | 0.53              |
| 34:BH:80:SER:O     | 34:BH:81:GLU:HB2    | 2.07                     | 0.53              |
| 37:BO:97:ARG:HB3   | 37:BO:99:PHE:HE1    | 1.72                     | 0.53              |
| 39:BQ:110:THR:O    | 39:BQ:113:GLN:N     | 2.42                     | 0.53              |
| 1:CA:1030(A):G:H3' | 1:CA:1030(B):C:H5'' | 1.90                     | 0.53              |
| 1:CA:1162:C:N3     | 1:CA:1175:G:C2      | 2.77                     | 0.53              |
| 1:CA:1315:U:C2'    | 1:CA:1316:G:H5'     | 2.39                     | 0.53              |
| 1:CA:15:G:H8       | 1:CA:1396:A:HO2'    | 1.55                     | 0.53              |
| 1:CA:276:G:O5'     | 1:CA:276:G:H8       | 1.92                     | 0.53              |
| 1:CA:390:C:H2'     | 1:CA:391:G:C8       | 2.44                     | 0.53              |
| 1:CA:720:C:H2'     | 1:CA:721:G:N7       | 2.23                     | 0.53              |
| 1:CA:954:G:H2'     | 1:CA:955:U:H6       | 1.73                     | 0.53              |
| 2:CB:36:ARG:N      | 2:CB:41:ILE:HD13    | 2.23                     | 0.53              |
| 4:CD:8:VAL:O       | 4:CD:11:LEU:HG      | 2.08                     | 0.53              |
| 5:CE:148:VAL:HG12  | 5:CE:152:ARG:NE     | 2.23                     | 0.53              |
| 5:CE:16:THR:O      | 5:CE:26:PHE:HD2     | 1.91                     | 0.53              |
| 5:CE:41:VAL:O      | 5:CE:66:MET:HA      | 2.09                     | 0.53              |
| 7:CG:80:VAL:HG21   | 7:CG:154:TYR:CE1    | 2.43                     | 0.53              |
| 1:CA:1344:C:H5'    | 9:CI:120:ARG:O      | 2.09                     | 0.53              |
| 12:CL:107:VAL:HG21 | 12:CL:117:TYR:HB3   | 1.90                     | 0.53              |
| 1:CA:1329:A:P      | 13:CM:28:ALA:HB3    | 2.49                     | 0.53              |
| 15:CO:36:ILE:HG22  | 15:CO:37:ASN:HD22   | 1.74                     | 0.53              |
| 19:CS:22:LEU:HD13  | 19:CS:27:GLU:CB     | 2.38                     | 0.53              |
| 19:CS:53:ASN:HD22  | 19:CS:77:THR:HA     | 1.73                     | 0.53              |
| 23:CW:4:G:H2'      | 23:CW:5:G:C8        | 2.44                     | 0.53              |
| 28:DB:13:A:OP2     | 49:D0:74:ARG:HG2    | 2.08                     | 0.53              |
| 50:D1:89:GLU:O     | 50:D1:92:LYS:HB3    | 2.08                     | 0.53              |
| 53:D4:60:GLU:O     | 53:D4:61:VAL:HB     | 2.09                     | 0.53              |
| 27:DA:1296:G:O2'   | 27:DA:1297:C:H5'    | 2.08                     | 0.53              |
| 27:DA:1321:A:H2'   | 27:DA:1322:A:C8     | 2.43                     | 0.53              |
| 27:DA:1651:G:N2    | 27:DA:1652:A:H1'    | 2.24                     | 0.53              |
| 27:DA:1718:G:N2    | 27:DA:1745:C:C2     | 2.76                     | 0.53              |
| 27:DA:1940:U:OP1   | 27:DA:1966:A:C2     | 2.61                     | 0.53              |
| 27:DA:1998:G:H2'   | 27:DA:1999:C:C6     | 2.44                     | 0.53              |
| 27:DA:2023:G:H5'   | 27:DA:2617:C:H4'    | 1.91                     | 0.53              |
| 27:DA:2108:C:C2'   | 27:DA:2109:U:H5'    | 2.38                     | 0.53              |
| 27:DA:2225:A:H4'   | 27:DA:2226:C:C6     | 2.43                     | 0.53              |
| 27:DA:2392:A:O2'   | 57:D8:27:THR:HB     | 2.09                     | 0.53              |
| 27:DA:25:U:C5      | 27:DA:26:G:C5       | 2.96                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:307:G:H21   | 27:DA:330:A:N6     | 2.07                     | 0.53              |
| 27:DA:311:A:O2'   | 27:DA:332:A:H5'    | 2.07                     | 0.53              |
| 27:DA:741:G:O2'   | 27:DA:742:G:H5'    | 2.08                     | 0.53              |
| 30:DD:132:PRO:HG3 | 30:DD:190:TYR:CE1  | 2.44                     | 0.53              |
| 32:DF:202:PHE:O   | 32:DF:203:GLN:C    | 2.47                     | 0.53              |
| 33:DG:111:LEU:CD2 | 33:DG:120:LEU:HD21 | 2.39                     | 0.53              |
| 33:DG:18:GLU:HG3  | 33:DG:22:ARG:HG3   | 1.90                     | 0.53              |
| 41:DS:53:SER:OG   | 41:DS:54:LEU:HD22  | 2.08                     | 0.53              |
| 44:DV:19:LYS:NZ   | 44:DV:20:LEU:N     | 2.56                     | 0.53              |
| 45:DW:107:LEU:N   | 45:DW:107:LEU:CD1  | 2.72                     | 0.53              |
| 1:AA:249:U:O5'    | 1:AA:249:U:H6      | 1.92                     | 0.53              |
| 1:AA:349:A:O2'    | 1:AA:350:G:H5'     | 2.09                     | 0.53              |
| 1:AA:593:G:H2'    | 1:AA:594:G:O4'     | 2.09                     | 0.53              |
| 3:AC:150:LYS:HA   | 3:AC:169:ALA:HA    | 1.91                     | 0.53              |
| 3:AC:175:LEU:O    | 3:AC:177:THR:N     | 2.41                     | 0.53              |
| 1:AA:1240:U:OP2   | 7:AG:116:ALA:HB2   | 2.09                     | 0.53              |
| 8:AH:17:THR:C     | 8:AH:19:VAL:H      | 2.11                     | 0.53              |
| 11:AK:12:ARG:CG   | 11:AK:13:GLN:N     | 2.71                     | 0.53              |
| 12:AL:34:CYS:CA   | 12:AL:55:VAL:HG22  | 2.39                     | 0.53              |
| 13:AM:3:ARG:HG2   | 13:AM:9:ILE:CG1    | 2.39                     | 0.53              |
| 17:AQ:87:LYS:HE2  | 17:AQ:87:LYS:CA    | 2.35                     | 0.53              |
| 18:AR:86:VAL:C    | 18:AR:87:ARG:HD3   | 2.28                     | 0.53              |
| 19:AS:22:LEU:HD13 | 19:AS:27:GLU:CB    | 2.39                     | 0.53              |
| 21:AU:6:ARG:HG2   | 21:AU:15:ARG:CZ    | 2.39                     | 0.53              |
| 50:B1:29:GLY:C    | 50:B1:30:VAL:HG13  | 2.29                     | 0.53              |
| 57:B8:49:VAL:CG2  | 57:B8:53:PRO:HB3   | 2.34                     | 0.53              |
| 27:BA:1119:C:O2'  | 27:BA:1120:G:H5'   | 2.08                     | 0.53              |
| 27:BA:1490:A:C5'  | 27:BA:1491:G:OP2   | 2.55                     | 0.53              |
| 27:BA:1556:C:O2'  | 27:BA:1557:C:H5'   | 2.08                     | 0.53              |
| 27:BA:186:G:H2'   | 27:BA:187:G:H8     | 1.73                     | 0.53              |
| 27:BA:1885:A:C8   | 27:BA:1885:A:H5'   | 2.42                     | 0.53              |
| 27:BA:205:G:O2'   | 27:BA:206:U:P      | 2.66                     | 0.53              |
| 27:BA:2098:U:H2'  | 27:BA:2099:U:C6    | 2.44                     | 0.53              |
| 27:BA:1786:A:H2   | 27:BA:2606:C:H1'   | 1.73                     | 0.53              |
| 27:BA:2626:C:H2'  | 27:BA:2627:G:O4'   | 2.09                     | 0.53              |
| 27:BA:2820:A:C8   | 31:BE:109:LYS:HE2  | 2.43                     | 0.53              |
| 27:BA:2863:C:OP1  | 42:BT:93:ARG:NH1   | 2.41                     | 0.53              |
| 27:BA:592:G:N3    | 57:B8:4:MET:CE     | 2.71                     | 0.53              |
| 27:BA:749:C:H2'   | 27:BA:749:C:O2     | 2.08                     | 0.53              |
| 27:BA:874:G:O2'   | 27:BA:875:G:H5'    | 2.08                     | 0.53              |
| 28:BB:55:U:H6     | 28:BB:55:U:O5'     | 1.92                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BD:164:GLN:OE1 | 30:BD:166:GLN:NE2  | 2.42                     | 0.53              |
| 30:BD:43:ARG:NH1  | 30:BD:44:ASN:OD1   | 2.39                     | 0.53              |
| 31:BE:6:GLY:HA2   | 31:BE:51:PHE:CZ    | 2.43                     | 0.53              |
| 32:BF:150:GLY:HA2 | 32:BF:172:TRP:CD2  | 2.44                     | 0.53              |
| 32:BF:202:PHE:HA  | 32:BF:205:ARG:CB   | 2.38                     | 0.53              |
| 39:BQ:10:ARG:HH11 | 39:BQ:10:ARG:HG3   | 1.72                     | 0.53              |
| 41:BS:41:ASP:OD2  | 41:BS:44:LYS:HB3   | 2.09                     | 0.53              |
| 42:BT:9:LEU:C     | 42:BT:11:GLU:H     | 2.10                     | 0.53              |
| 1:CA:1028:C:H2'   | 1:CA:1029:C:H5'    | 1.90                     | 0.53              |
| 1:CA:1512:U:H2'   | 1:CA:1513:A:C8     | 2.44                     | 0.53              |
| 1:CA:218:C:HO2'   | 1:CA:219:C:H6      | 1.55                     | 0.53              |
| 1:CA:254:G:C2'    | 1:CA:255:G:H5'     | 2.39                     | 0.53              |
| 1:CA:336:C:C2'    | 1:CA:337:C:H5'     | 2.38                     | 0.53              |
| 1:CA:409:G:C2     | 1:CA:410:G:H1'     | 2.43                     | 0.53              |
| 1:CA:438:G:N2     | 1:CA:494:U:H3'     | 2.23                     | 0.53              |
| 1:CA:658:G:C6     | 1:CA:659:U:C4      | 2.96                     | 0.53              |
| 1:CA:838:G:H2'    | 1:CA:839:U:C5'     | 2.35                     | 0.53              |
| 1:CA:913:A:H1'    | 1:CA:914:A:O4'     | 2.09                     | 0.53              |
| 1:CA:826:C:H5'    | 8:CH:12:ARG:NH2    | 2.24                     | 0.53              |
| 9:CI:79:LEU:HD21  | 9:CI:102:LEU:HD22  | 1.89                     | 0.53              |
| 11:CK:127:LYS:CA  | 11:CK:127:LYS:HE2  | 2.36                     | 0.53              |
| 13:CM:58:GLU:HA   | 13:CM:58:GLU:OE1   | 2.09                     | 0.53              |
| 17:CQ:45:HIS:O    | 17:CQ:73:VAL:HG23  | 2.09                     | 0.53              |
| 18:CR:58:LEU:HD23 | 18:CR:62:GLU:HB3   | 1.91                     | 0.53              |
| 19:CS:17:GLU:O    | 19:CS:20:LEU:HB2   | 2.08                     | 0.53              |
| 23:CW:31:U:H6     | 23:CW:31:U:H5'     | 1.74                     | 0.53              |
| 27:DA:61:G:H5'    | 51:D2:50:ILE:HD12  | 1.91                     | 0.53              |
| 51:D2:54:LYS:O    | 51:D2:57:ILE:HB    | 2.09                     | 0.53              |
| 52:D3:58:VAL:O    | 52:D3:58:VAL:HG12  | 2.08                     | 0.53              |
| 56:D7:41:ARG:CB   | 56:D7:41:ARG:NH1   | 2.52                     | 0.53              |
| 57:D8:33:ASN:H    | 57:D8:33:ASN:ND2   | 2.05                     | 0.53              |
| 57:D8:16:ILE:HG21 | 57:D8:64:TYR:HB3   | 1.90                     | 0.53              |
| 27:DA:182:A:O2'   | 27:DA:183:C:H5'    | 2.08                     | 0.53              |
| 27:DA:1971:A:H2   | 30:DD:239:ARG:O    | 1.92                     | 0.53              |
| 27:DA:2020:A:O2'  | 27:DA:2021:C:H5'   | 2.09                     | 0.53              |
| 27:DA:2050:C:H2'  | 27:DA:2051:A:O4'   | 2.08                     | 0.53              |
| 27:DA:2233:U:H2'  | 27:DA:2234:G:C8    | 2.43                     | 0.53              |
| 29:DC:41:VAL:HA   | 29:DC:213:TYR:HA   | 1.90                     | 0.53              |
| 30:DD:90:ALA:HB1  | 30:DD:106:ILE:HG13 | 1.90                     | 0.53              |
| 30:DD:32:SER:HA   | 30:DD:36:PRO:CD    | 2.38                     | 0.53              |
| 27:DA:2772:C:OP1  | 31:DE:202:LYS:HE2  | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DE:26:ILE:CG2   | 31:DE:27:LEU:H     | 2.07                     | 0.53              |
| 31:DE:48:GLN:CD    | 31:DE:78:LEU:HD12  | 2.29                     | 0.53              |
| 27:DA:2810:A:H2'   | 31:DE:61:ARG:NH2   | 2.23                     | 0.53              |
| 33:DG:105:LYS:HD2  | 33:DG:143:GLU:OE1  | 2.08                     | 0.53              |
| 36:DN:19:GLU:HB2   | 36:DN:59:LYS:CB    | 2.39                     | 0.53              |
| 36:DN:76:SER:O     | 36:DN:78:TYR:HD1   | 1.92                     | 0.53              |
| 37:DO:15:GLY:HA3   | 37:DO:50:GLY:HA3   | 1.89                     | 0.53              |
| 39:DQ:58:PHE:CD1   | 39:DQ:61:GLY:HA3   | 2.44                     | 0.53              |
| 41:DS:101:LEU:CD2  | 41:DS:104:GLY:H    | 2.21                     | 0.53              |
| 41:DS:97:ARG:O     | 41:DS:98:VAL:C     | 2.47                     | 0.53              |
| 45:DW:18:ARG:HG2   | 45:DW:76:VAL:CG1   | 2.38                     | 0.53              |
| 47:DY:81:LYS:O     | 47:DY:82:PRO:O     | 2.26                     | 0.53              |
| 48:DZ:29:ASN:O     | 48:DZ:30:ARG:CB    | 2.57                     | 0.53              |
| 1:AA:1257:U:H3'    | 1:AA:1257:U:C6     | 2.42                     | 0.53              |
| 1:AA:1263:C:H2'    | 1:AA:1264:C:H5'    | 1.91                     | 0.53              |
| 1:AA:1239:A:N6     | 1:AA:1299:A:H62    | 2.03                     | 0.53              |
| 1:AA:1371:G:H2'    | 1:AA:1372:U:H6     | 1.72                     | 0.53              |
| 1:AA:1442(A):G:C4' | 1:AA:1442(B):A:OP2 | 2.55                     | 0.53              |
| 1:AA:747:C:OP2     | 1:AA:748:C:N4      | 2.42                     | 0.53              |
| 1:AA:874:G:H2'     | 1:AA:875:C:C6      | 2.44                     | 0.53              |
| 2:AB:168:THR:CG2   | 2:AB:192:SER:HA    | 2.38                     | 0.53              |
| 2:AB:29:ALA:O      | 2:AB:32:ILE:HG22   | 2.08                     | 0.53              |
| 3:AC:6:HIS:HD2     | 3:AC:8:ILE:H       | 1.57                     | 0.53              |
| 4:AD:141:ARG:O     | 4:AD:144:ASP:OD2   | 2.27                     | 0.53              |
| 6:AF:19:LEU:HD11   | 6:AF:59:TYR:CE1    | 2.43                     | 0.53              |
| 7:AG:113:GLU:O     | 7:AG:119:ARG:HD3   | 2.09                     | 0.53              |
| 8:AH:77:GLU:HG2    | 8:AH:78:GLN:N      | 2.22                     | 0.53              |
| 9:AI:4:TYR:HA      | 9:AI:88:TYR:CD1    | 2.44                     | 0.53              |
| 10:AJ:84:GLN:H     | 10:AJ:84:GLN:CD    | 2.13                     | 0.53              |
| 11:AK:88:GLY:O     | 11:AK:90:GLY:N     | 2.40                     | 0.53              |
| 1:AA:280:C:O2      | 17:AQ:38:ARG:HG3   | 2.08                     | 0.53              |
| 17:AQ:76:LEU:HD12  | 17:AQ:77:VAL:N     | 2.23                     | 0.53              |
| 19:AS:43:GLU:C     | 19:AS:45:VAL:H     | 2.12                     | 0.53              |
| 27:BA:2271:G:C4'   | 49:B0:20:ARG:NH1   | 2.67                     | 0.53              |
| 49:B0:33:ALA:HB2   | 49:B0:63:VAL:HA    | 1.91                     | 0.53              |
| 53:B4:40:ILE:O     | 53:B4:41:ILE:HD13  | 2.08                     | 0.53              |
| 27:BA:1358:G:O2'   | 27:BA:1359:A:H5''  | 2.09                     | 0.53              |
| 27:BA:152:G:H2'    | 27:BA:153:C:O4'    | 2.08                     | 0.53              |
| 27:BA:1817:G:H2'   | 27:BA:1818:U:H5'   | 1.91                     | 0.53              |
| 27:BA:2074:U:H2'   | 27:BA:2075:U:C6    | 2.43                     | 0.53              |
| 27:BA:2078:C:O2'   | 27:BA:2079:U:H5'   | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2095:C:H2'   | 27:BA:2096:U:C6    | 2.44                     | 0.53              |
| 27:BA:466:A:O4'    | 27:BA:683:C:H4'    | 2.09                     | 0.53              |
| 28:BB:109:C:H5'    | 28:BB:110:G:O5'    | 2.09                     | 0.53              |
| 28:BB:21:G:H2'     | 28:BB:22:U:C6      | 2.43                     | 0.53              |
| 30:BD:270:ILE:HD12 | 30:BD:271:ILE:N    | 2.24                     | 0.53              |
| 32:BF:4:VAL:HB     | 32:BF:17:ARG:HE    | 1.73                     | 0.53              |
| 33:BG:52:ILE:HG22  | 33:BG:54:GLU:CG    | 2.38                     | 0.53              |
| 34:BH:37:VAL:O     | 34:BH:38:SER:C     | 2.47                     | 0.53              |
| 27:BA:2758:A:C4    | 34:BH:67:LEU:HD21  | 2.44                     | 0.53              |
| 27:BA:558:G:OP2    | 36:BN:111:PRO:HD2  | 2.09                     | 0.53              |
| 37:BO:116:SER:OG   | 37:BO:117:LEU:N    | 2.42                     | 0.53              |
| 38:BP:101:VAL:HG13 | 38:BP:106:LEU:HD23 | 1.90                     | 0.53              |
| 38:BP:23:PRO:CD    | 38:BP:33:ARG:NH2   | 2.72                     | 0.53              |
| 38:BP:61:ARG:H     | 38:BP:61:ARG:CD    | 2.20                     | 0.53              |
| 38:BP:92:GLU:HB2   | 38:BP:121:LYS:NZ   | 2.24                     | 0.53              |
| 39:BQ:79:LEU:O     | 39:BQ:81:VAL:HG12  | 2.07                     | 0.53              |
| 27:BA:1654:A:P     | 40:BR:3:HIS:HB2    | 2.49                     | 0.53              |
| 27:BA:748:G:C8     | 45:BW:89:ALA:CB    | 2.92                     | 0.53              |
| 47:BY:84:ARG:O     | 47:BY:95:LYS:N     | 2.29                     | 0.53              |
| 1:CA:1206:G:H4'    | 3:CC:192:THR:C     | 2.29                     | 0.53              |
| 5:CE:101:ILE:CG1   | 5:CE:119:LEU:HD23  | 2.38                     | 0.53              |
| 5:CE:32:VAL:O      | 5:CE:43:LEU:HD12   | 2.08                     | 0.53              |
| 6:CF:75:LEU:HD23   | 6:CF:79:LEU:HD11   | 1.91                     | 0.53              |
| 6:CF:74:ASP:O      | 6:CF:77:ARG:HB3    | 2.09                     | 0.53              |
| 6:CF:82:ARG:HB2    | 6:CF:85:VAL:CG2    | 2.38                     | 0.53              |
| 8:CH:7:ALA:CA      | 8:CH:85:ARG:HG3    | 2.38                     | 0.53              |
| 9:CI:127:LYS:O     | 9:CI:127:LYS:HG2   | 2.09                     | 0.53              |
| 11:CK:78:GLN:O     | 11:CK:103:LEU:CD1  | 2.56                     | 0.53              |
| 12:CL:66:TYR:CD2   | 12:CL:67:ILE:N     | 2.70                     | 0.53              |
| 20:CT:23:ARG:O     | 20:CT:26:ASN:ND2   | 2.42                     | 0.53              |
| 24:CX:51:C:H2'     | 24:CX:52:G:C8      | 2.34                     | 0.53              |
| 24:CX:52:G:O2'     | 24:CX:53:G:H5'     | 2.08                     | 0.53              |
| 27:DA:2231:C:OP1   | 50:D1:42:GLN:HA    | 2.07                     | 0.53              |
| 50:D1:66:HIS:C     | 50:D1:68:PRO:HD2   | 2.30                     | 0.53              |
| 55:D6:15:GLU:OE1   | 55:D6:43:CYS:SG    | 2.67                     | 0.53              |
| 27:DA:1344:G:OP1   | 27:DA:1345:C:H5    | 1.91                     | 0.53              |
| 27:DA:1669:A:H2    | 27:DA:1994:C:H1'   | 1.72                     | 0.53              |
| 27:DA:2075:U:C5    | 27:DA:2238:G:C5    | 2.96                     | 0.53              |
| 27:DA:2361:A:OP1   | 57:D8:26:LYS:HD3   | 2.09                     | 0.53              |
| 27:DA:2846:G:H2'   | 27:DA:2847:U:H6    | 1.74                     | 0.53              |
| 27:DA:727:A:H2'    | 27:DA:728:G:C8     | 2.44                     | 0.53              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 27:DA:940:G:C3'    | 27:DA:941:A:H5'' | 2.38                     | 0.53              |
| 27:DA:996:A:H4'    | 43:DU:92:ARG:NH2 | 2.24                     | 0.53              |
| 29:DC:72:VAL:HG21  | 29:DC:161:ILE:HA | 1.91                     | 0.53              |
| 32:DF:141:ALA:O    | 32:DF:144:LYS:N  | 2.42                     | 0.53              |
| 32:DF:57:VAL:HG11  | 32:DF:59:TYR:CD1 | 2.43                     | 0.53              |
| 33:DG:16:ARG:N     | 33:DG:17:PRO:CD  | 2.72                     | 0.53              |
| 38:DP:105:LEU:HD23 | 38:DP:105:LEU:N  | 2.24                     | 0.53              |
| 39:DQ:85:LYS:HG3   | 49:D0:7:LEU:HD22 | 1.90                     | 0.53              |
| 40:DR:55:ALA:HA    | 40:DR:80:PHE:CE1 | 2.43                     | 0.53              |
| 42:DT:50:ILE:HG21  | 42:DT:100:TYR:HA | 1.91                     | 0.53              |
| 44:DV:19:LYS:HB3   | 44:DV:94:LEU:O   | 2.09                     | 0.53              |
| 46:DX:69:TYR:CD1   | 46:DX:69:TYR:N   | 2.77                     | 0.53              |
| 48:DZ:95:VAL:HG12  | 48:DZ:96:GLU:N   | 2.24                     | 0.53              |
| 1:AA:1072:G:C2'    | 1:AA:1073:U:H5'  | 2.39                     | 0.53              |
| 1:AA:1270:C:H2'    | 1:AA:1271:G:O4'  | 2.08                     | 0.53              |
| 1:AA:1314:C:H5     | 19:AS:6:LYS:HZ3  | 1.57                     | 0.53              |
| 1:AA:245:C:O2      | 1:AA:283:C:N3    | 2.42                     | 0.53              |
| 1:AA:486:U:O2'     | 1:AA:487:A:H8    | 1.74                     | 0.53              |
| 1:AA:644:G:H2'     | 1:AA:645:C:H5'   | 1.89                     | 0.53              |
| 2:AB:64:ARG:O      | 2:AB:64:ARG:HG3  | 2.08                     | 0.53              |
| 3:AC:42:LEU:N      | 3:AC:45:LYS:HZ3  | 2.07                     | 0.53              |
| 3:AC:77:ILE:C      | 3:AC:83:ARG:HB3  | 2.30                     | 0.53              |
| 5:AE:90:VAL:O      | 5:AE:91:LEU:HD13 | 2.09                     | 0.53              |
| 7:AG:86:GLN:NE2    | 25:AY:30:A:H2    | 2.06                     | 0.53              |
| 11:AK:16:SER:O     | 11:AK:35:PRO:HD3 | 2.08                     | 0.53              |
| 18:AR:63:GLN:OE1   | 18:AR:63:GLN:HA  | 2.09                     | 0.53              |
| 19:AS:45:VAL:C     | 19:AS:47:HIS:H   | 2.12                     | 0.53              |
| 20:AT:67:ALA:HA    | 20:AT:72:LEU:O   | 2.09                     | 0.53              |
| 1:AA:1305:G:H5'    | 21:AU:4:GLY:HA3  | 1.91                     | 0.53              |
| 25:AY:28:G:O2'     | 25:AY:29:G:H5'   | 2.09                     | 0.53              |
| 56:B7:9:ARG:O      | 56:B7:10:ARG:C   | 2.46                     | 0.53              |
| 27:BA:1207:C:H2'   | 27:BA:1208:C:H6  | 1.74                     | 0.53              |
| 27:BA:1388:G:O2'   | 27:BA:1389:G:H5' | 2.08                     | 0.53              |
| 27:BA:1486:A:H2'   | 27:BA:1487:G:H8  | 1.74                     | 0.53              |
| 27:BA:1688:U:O2    | 27:BA:1700:A:H5' | 2.09                     | 0.53              |
| 27:BA:2097:C:H2'   | 27:BA:2098:U:C6  | 2.43                     | 0.53              |
| 27:BA:2360:A:H2'   | 27:BA:2361:A:O4' | 2.09                     | 0.53              |
| 27:BA:2346:A:C8    | 27:BA:2383:G:C4  | 2.97                     | 0.53              |
| 27:BA:2392:A:C2    | 27:BA:2429:G:C2  | 2.97                     | 0.53              |
| 27:BA:2580:U:C5'   | 31:BE:131:ALA:H  | 2.22                     | 0.53              |
| 27:BA:2882:A:H5'   | 40:BR:96:ARG:HG3 | 1.90                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:492:A:C2     | 27:BA:493:G:H1'   | 2.44                     | 0.53              |
| 27:BA:681:G:H2'    | 27:BA:682:G:H8    | 1.73                     | 0.53              |
| 27:BA:747:U:N1     | 54:B5:2:ALA:N     | 2.57                     | 0.53              |
| 27:BA:83:G:C2'     | 27:BA:84:A:OP2    | 2.57                     | 0.53              |
| 27:BA:1819:A:C2'   | 30:BD:178:PRO:HB2 | 2.38                     | 0.53              |
| 30:BD:211:ARG:HD3  | 30:BD:214:TRP:CZ3 | 2.44                     | 0.53              |
| 30:BD:58:HIS:HD2   | 30:BD:59:LYS:O    | 1.92                     | 0.53              |
| 32:BF:110:LEU:HD21 | 32:BF:181:LEU:HG  | 1.91                     | 0.53              |
| 32:BF:184:TYR:O    | 32:BF:188:ARG:CB  | 2.57                     | 0.53              |
| 32:BF:184:TYR:CE2  | 32:BF:188:ARG:HD2 | 2.43                     | 0.53              |
| 34:BH:139:GLN:HG3  | 34:BH:140:LYS:N   | 2.24                     | 0.53              |
| 37:BO:66:LYS:H     | 37:BO:82:ASN:ND2  | 2.06                     | 0.53              |
| 38:BP:144:GLU:H    | 38:BP:145:PRO:CD  | 2.17                     | 0.53              |
| 39:BQ:57:HIS:CE1   | 39:BQ:116:GLU:CG  | 2.92                     | 0.53              |
| 40:BR:23:ASN:HD22  | 40:BR:23:ASN:N    | 2.06                     | 0.53              |
| 1:AA:1432:G:OP1    | 42:BT:107:ASP:HB2 | 2.09                     | 0.53              |
| 43:BU:24:TYR:HB2   | 43:BU:29:SER:HB3  | 1.91                     | 0.53              |
| 44:BV:64:HIS:HB3   | 44:BV:91:TYR:O    | 2.09                     | 0.53              |
| 46:BX:25:LYS:HG2   | 46:BX:80:ILE:HD11 | 1.91                     | 0.53              |
| 47:BY:87:LYS:CG    | 47:BY:88:LYS:N    | 2.72                     | 0.53              |
| 1:CA:170:U:O2'     | 1:CA:171:A:H5'    | 2.09                     | 0.53              |
| 1:CA:376:G:H1      | 1:CA:387:U:H3     | 1.57                     | 0.53              |
| 1:CA:471:G:O2'     | 1:CA:472:A:O5'    | 2.27                     | 0.53              |
| 1:CA:59:A:H2'      | 1:CA:59:A:N3      | 2.22                     | 0.53              |
| 1:CA:707:C:C2      | 1:CA:708:C:C5     | 2.97                     | 0.53              |
| 1:CA:735:C:H6      | 1:CA:735:C:O5'    | 1.91                     | 0.53              |
| 1:CA:956:U:H2'     | 1:CA:957:U:O4'    | 2.09                     | 0.53              |
| 10:CJ:58:ASP:O     | 10:CJ:59:SER:C    | 2.47                     | 0.53              |
| 12:CL:41:THR:HG21  | 26:CZ:6:5OH:HR    | 1.91                     | 0.53              |
| 14:CN:47:LEU:O     | 14:CN:50:LYS:N    | 2.42                     | 0.53              |
| 12:CL:5:ASN:ND2    | 17:CQ:34:LYS:NZ   | 2.56                     | 0.53              |
| 24:CX:47:U:H3'     | 24:CX:48:C:C5'    | 2.38                     | 0.53              |
| 26:CZ:5:UAL:C      | 26:CZ:6:5OH:HS    | 2.39                     | 0.53              |
| 57:D8:63:PRO:HB2   | 57:D8:64:TYR:HD1  | 1.74                     | 0.53              |
| 27:DA:2083:G:H2'   | 27:DA:2084:C:C6   | 2.44                     | 0.53              |
| 27:DA:2222:G:H5'   | 30:DD:149:PRO:HG3 | 1.90                     | 0.53              |
| 27:DA:194:G:N2     | 27:DA:251:A:H2    | 2.07                     | 0.53              |
| 27:DA:2601:C:H6    | 27:DA:2601:C:O5'  | 1.92                     | 0.53              |
| 27:DA:10:G:N1      | 27:DA:2629:A:H1'  | 2.24                     | 0.53              |
| 27:DA:477:A:O2'    | 27:DA:478:A:C8    | 2.59                     | 0.53              |
| 27:DA:606:U:H4'    | 27:DA:658:C:H4'   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DD:77:ALA:HB2  | 30:DD:97:TYR:CD2  | 2.44                     | 0.53              |
| 31:DE:16:ARG:NH1  | 31:DE:171:GLU:OE2 | 2.41                     | 0.53              |
| 33:DG:51:ARG:NE   | 33:DG:51:ARG:CA   | 2.70                     | 0.53              |
| 34:DH:44:VAL:HG12 | 34:DH:45:VAL:N    | 2.16                     | 0.53              |
| 38:DP:80:TYR:HA   | 38:DP:111:ARG:O   | 2.09                     | 0.53              |
| 38:DP:33:ARG:O    | 38:DP:35:HIS:N    | 2.42                     | 0.53              |
| 38:DP:9:ASN:H     | 38:DP:10:PRO:HD2  | 1.74                     | 0.53              |
| 42:DT:129:ARG:HG3 | 42:DT:129:ARG:O   | 2.08                     | 0.53              |
| 46:DX:26:TYR:OH   | 46:DX:89:ILE:N    | 2.37                     | 0.53              |
| 47:DY:17:SER:OG   | 47:DY:18:GLY:N    | 2.42                     | 0.53              |
| 47:DY:75:ILE:CB   | 47:DY:80:GLY:H    | 2.21                     | 0.53              |
| 27:DA:298:G:P     | 47:DY:85:VAL:HG23 | 2.49                     | 0.53              |
| 48:DZ:102:ARG:HD3 | 48:DZ:135:PHE:CZ  | 2.44                     | 0.53              |
| 1:AA:1053:G:N7    | 1:AA:1199:U:H3'   | 2.24                     | 0.52              |
| 1:AA:1072:G:H2'   | 1:AA:1073:U:O4'   | 2.08                     | 0.52              |
| 1:AA:1248:A:H2'   | 1:AA:1249:C:C5'   | 2.39                     | 0.52              |
| 1:AA:1333:A:H2'   | 1:AA:1334:G:O4'   | 2.08                     | 0.52              |
| 1:AA:1472:U:C2'   | 1:AA:1473:A:H5'   | 2.39                     | 0.52              |
| 1:AA:243:A:H4'    | 1:AA:244:U:C5'    | 2.39                     | 0.52              |
| 1:AA:558:G:H2'    | 1:AA:559:A:H2     | 1.73                     | 0.52              |
| 2:AB:185:ILE:HG12 | 2:AB:199:TYR:HB2  | 1.91                     | 0.52              |
| 4:AD:13:ARG:O     | 4:AD:14:ARG:HB3   | 2.08                     | 0.52              |
| 5:AE:33:VAL:HA    | 5:AE:42:GLY:O     | 2.08                     | 0.52              |
| 6:AF:24:GLU:CG    | 6:AF:25:ILE:N     | 2.71                     | 0.52              |
| 6:AF:7:ASN:C      | 6:AF:8:ILE:HG13   | 2.29                     | 0.52              |
| 9:AI:127:LYS:O    | 9:AI:128:ARG:HB3  | 2.08                     | 0.52              |
| 12:AL:31:ARG:HG3  | 12:AL:102:TYR:CE1 | 2.44                     | 0.52              |
| 1:AA:1228:C:H4'   | 13:AM:116:THR:HA  | 1.92                     | 0.52              |
| 13:AM:76:ALA:HA   | 13:AM:79:LYS:CD   | 2.38                     | 0.52              |
| 14:AN:24:CYS:HB2  | 14:AN:29:ARG:HB3  | 1.92                     | 0.52              |
| 49:B0:50:ASN:HA   | 49:B0:62:LEU:HD12 | 1.92                     | 0.52              |
| 57:B8:6:THR:CA    | 57:B8:61:LEU:HD11 | 2.35                     | 0.52              |
| 58:B9:11:CYS:SG   | 58:B9:32:HIS:CG   | 3.02                     | 0.52              |
| 27:BA:1359:A:N7   | 27:BA:1372:U:O4   | 2.42                     | 0.52              |
| 27:BA:1444:G:C6   | 27:BA:1466:G:N1   | 2.77                     | 0.52              |
| 27:BA:1508:A:H2'  | 27:BA:1508:A:N3   | 2.23                     | 0.52              |
| 27:BA:2289:G:C2'  | 27:BA:2290:G:H5'' | 2.38                     | 0.52              |
| 27:BA:2371:G:H4'  | 55:B6:45:LYS:CB   | 2.39                     | 0.52              |
| 27:BA:945:A:C4    | 27:BA:2448:A:C2   | 2.96                     | 0.52              |
| 27:BA:2548:G:H1   | 27:BA:2560:C:H42  | 1.55                     | 0.52              |
| 27:BA:394:A:C6    | 27:BA:395:U:N3    | 2.77                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:721:C:H2'    | 27:BA:722:A:H8     | 1.73                     | 0.52              |
| 27:BA:863:A:H2'    | 27:BA:864:G:H8     | 1.69                     | 0.52              |
| 30:BD:10:THR:HG23  | 30:BD:13:ARG:CB    | 2.38                     | 0.52              |
| 30:BD:52:ARG:NH1   | 30:BD:249:PRO:HG2  | 2.23                     | 0.52              |
| 32:BF:3:GLU:HA     | 32:BF:24:LEU:HB3   | 1.90                     | 0.52              |
| 33:BG:11:TYR:O     | 33:BG:16:ARG:N     | 2.36                     | 0.52              |
| 33:BG:170:ARG:HH21 | 33:BG:182:LYS:HZ3  | 1.55                     | 0.52              |
| 37:BO:13:ASN:HD21  | 37:BO:96:THR:H     | 1.53                     | 0.52              |
| 37:BO:10:VAL:CG2   | 37:BO:17:ARG:HA    | 2.39                     | 0.52              |
| 39:BQ:17:LEU:HD21  | 39:BQ:41:TRP:HE1   | 1.73                     | 0.52              |
| 41:BS:103:GLU:O    | 41:BS:104:GLY:C    | 2.47                     | 0.52              |
| 41:BS:40:ILE:CG2   | 41:BS:41:ASP:N     | 2.71                     | 0.52              |
| 41:BS:95:HIS:CG    | 41:BS:96:GLY:H     | 2.26                     | 0.52              |
| 48:BZ:79:ARG:O     | 48:BZ:81:ARG:N     | 2.41                     | 0.52              |
| 1:CA:186:C:H2'     | 1:CA:187:C:H6      | 1.74                     | 0.52              |
| 1:CA:429:U:OP2     | 4:CD:36:ARG:NH1    | 2.42                     | 0.52              |
| 1:CA:742:G:H5'     | 15:CO:58:MET:CE    | 2.39                     | 0.52              |
| 1:CA:949:A:H2'     | 1:CA:950:U:O4'     | 2.08                     | 0.52              |
| 1:CA:9:G:H5'       | 5:CE:122:GLU:CD    | 2.28                     | 0.52              |
| 6:CF:10:LEU:O      | 6:CF:11:ASN:C      | 2.46                     | 0.52              |
| 8:CH:36:LEU:O      | 8:CH:37:ARG:C      | 2.46                     | 0.52              |
| 8:CH:7:ALA:HA      | 8:CH:85:ARG:HG3    | 1.90                     | 0.52              |
| 8:CH:88:LYS:HB3    | 8:CH:89:PRO:HD2    | 1.90                     | 0.52              |
| 10:CJ:40:LEU:HG    | 10:CJ:69:ASN:CB    | 2.37                     | 0.52              |
| 11:CK:99:GLN:OE1   | 11:CK:105:VAL:HG21 | 2.09                     | 0.52              |
| 12:CL:123:LYS:HD2  | 12:CL:124:GLU:H    | 1.74                     | 0.52              |
| 52:D3:6:VAL:HB     | 52:D3:54:VAL:HG11  | 1.91                     | 0.52              |
| 56:D7:42:LEU:HD23  | 56:D7:42:LEU:N     | 2.23                     | 0.52              |
| 57:D8:28:GLY:O     | 57:D8:29:LYS:HB3   | 2.08                     | 0.52              |
| 27:DA:1281:G:C2    | 27:DA:1290:C:N3    | 2.76                     | 0.52              |
| 27:DA:1567:A:C2    | 30:DD:84:TYR:HB3   | 2.44                     | 0.52              |
| 27:DA:1941:C:C5    | 27:DA:1942:C:C5    | 2.98                     | 0.52              |
| 27:DA:197:A:H8     | 27:DA:197:A:H5'    | 1.71                     | 0.52              |
| 27:DA:2199:A:H3'   | 27:DA:2200:C:C6    | 2.33                     | 0.52              |
| 27:DA:2836:U:C4    | 27:DA:2883:A:N6    | 2.78                     | 0.52              |
| 27:DA:325:G:H2'    | 27:DA:326:G:H8     | 1.74                     | 0.52              |
| 27:DA:635:C:H2'    | 27:DA:636:G:H8     | 1.74                     | 0.52              |
| 27:DA:859:G:N2     | 27:DA:916:G:H2'    | 2.25                     | 0.52              |
| 29:DC:83:ILE:HA    | 29:DC:94:VAL:CG2   | 2.36                     | 0.52              |
| 30:DD:158:ALA:HB3  | 30:DD:161:THR:HG21 | 1.91                     | 0.52              |
| 27:DA:2621:A:O2'   | 31:DE:159:HIS:HB2  | 2.10                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DE:119:ARG:HG3  | 31:DE:160:TYR:HB2  | 1.92                     | 0.52              |
| 33:DG:111:LEU:HD22 | 33:DG:117:PHE:CE1  | 2.44                     | 0.52              |
| 42:DT:81:PRO:O     | 42:DT:82:LEU:HD12  | 2.09                     | 0.52              |
| 43:DU:70:ARG:C     | 43:DU:72:HIS:H     | 2.12                     | 0.52              |
| 44:DV:21:ARG:HG2   | 44:DV:91:TYR:CD1   | 2.43                     | 0.52              |
| 48:DZ:156:LEU:N    | 48:DZ:156:LEU:HD12 | 2.24                     | 0.52              |
| 1:AA:1104:G:H4'    | 2:AB:111:ARG:NH1   | 2.23                     | 0.52              |
| 1:AA:1247:U:O2     | 1:AA:1291:G:C2     | 2.62                     | 0.52              |
| 1:AA:1327:C:OP1    | 21:AU:20:LYS:HB3   | 2.09                     | 0.52              |
| 1:AA:1347:G:O2'    | 1:AA:1348:U:P      | 2.67                     | 0.52              |
| 1:AA:252:U:H2'     | 1:AA:253:U:H5'     | 1.91                     | 0.52              |
| 1:AA:329:A:C5      | 1:AA:332:G:C6      | 2.98                     | 0.52              |
| 3:AC:52:LEU:CD2    | 3:AC:52:LEU:N      | 2.66                     | 0.52              |
| 7:AG:152:ALA:C     | 7:AG:154:TYR:H     | 2.11                     | 0.52              |
| 9:AI:11:LYS:O      | 9:AI:13:ALA:N      | 2.42                     | 0.52              |
| 50:B1:37:ILE:O     | 50:B1:38:SER:CB    | 2.57                     | 0.52              |
| 27:BA:1003:G:N2    | 27:BA:1153:C:C2    | 2.78                     | 0.52              |
| 27:BA:1280:G:N2    | 27:BA:1281:G:H1'   | 2.24                     | 0.52              |
| 27:BA:1830:C:O2'   | 27:BA:1831:G:H5'   | 2.08                     | 0.52              |
| 27:BA:196:A:O4'    | 38:BP:46:LYS:HE3   | 2.09                     | 0.52              |
| 27:BA:2271:G:OP1   | 49:B0:18:ALA:HB1   | 2.09                     | 0.52              |
| 27:BA:2545:G:H2'   | 27:BA:2546:U:O4'   | 2.09                     | 0.52              |
| 27:BA:2607:G:O2'   | 27:BA:2608:G:H5'   | 2.10                     | 0.52              |
| 27:BA:525:U:H6     | 27:BA:525:U:OP2    | 1.91                     | 0.52              |
| 27:BA:646:A:H2'    | 27:BA:647:G:O4'    | 2.10                     | 0.52              |
| 27:BA:671:C:H5'    | 27:BA:671:C:H6     | 1.75                     | 0.52              |
| 27:BA:857:C:O2     | 27:BA:857:C:H2'    | 2.08                     | 0.52              |
| 27:BA:937:U:C4     | 27:BA:938:G:N7     | 2.78                     | 0.52              |
| 30:BD:45:ASN:CG    | 30:BD:46:GLN:H     | 2.13                     | 0.52              |
| 31:BE:143:ASN:HB2  | 31:BE:147:PRO:HD2  | 1.91                     | 0.52              |
| 33:BG:138:GLN:HB3  | 33:BG:153:ARG:O    | 2.08                     | 0.52              |
| 35:BI:40:THR:OG1   | 35:BI:43:ASN:ND2   | 2.42                     | 0.52              |
| 35:BI:77:LEU:CD2   | 35:BI:78:THR:N     | 2.71                     | 0.52              |
| 39:BQ:79:LEU:N     | 39:BQ:79:LEU:CD1   | 2.71                     | 0.52              |
| 41:BS:33:LYS:O     | 41:BS:34:HIS:CG    | 2.63                     | 0.52              |
| 27:BA:584:C:OP2    | 43:BU:6:THR:HB     | 2.10                     | 0.52              |
| 45:BW:29:LEU:HD21  | 45:BW:33:ARG:NH2   | 2.24                     | 0.52              |
| 1:CA:1117:G:N2     | 1:CA:1180:A:H1'    | 2.25                     | 0.52              |
| 1:CA:1209:C:H2'    | 1:CA:1209:C:O2     | 2.07                     | 0.52              |
| 1:CA:1347:G:N2     | 1:CA:1373:G:C2'    | 2.58                     | 0.52              |
| 1:CA:1349:A:H2'    | 1:CA:1350:A:C8     | 2.45                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:158:G:C2'     | 1:CA:159:G:H5'    | 2.39                     | 0.52              |
| 1:CA:181:G:N2      | 1:CA:183:G:H1     | 2.07                     | 0.52              |
| 1:CA:250:A:C2      | 1:CA:274:A:N6     | 2.77                     | 0.52              |
| 1:CA:375:U:H2'     | 1:CA:376:G:C8     | 2.44                     | 0.52              |
| 1:CA:505:G:H2'     | 1:CA:506:G:C8     | 2.45                     | 0.52              |
| 1:CA:701:C:O2'     | 1:CA:703:G:C6     | 2.60                     | 0.52              |
| 2:CB:16:HIS:CE1    | 2:CB:213:LEU:HD13 | 2.43                     | 0.52              |
| 2:CB:36:ARG:CA     | 2:CB:36:ARG:NE    | 2.72                     | 0.52              |
| 3:CC:76:VAL:HG23   | 3:CC:77:ILE:H     | 1.75                     | 0.52              |
| 5:CE:135:THR:O     | 5:CE:136:MET:C    | 2.48                     | 0.52              |
| 5:CE:7:GLU:O       | 5:CE:8:GLU:CB     | 2.57                     | 0.52              |
| 6:CF:2:ARG:O       | 6:CF:66:GLU:HA    | 2.09                     | 0.52              |
| 6:CF:99:ALA:O      | 6:CF:100:ASN:C    | 2.48                     | 0.52              |
| 9:CI:62:TYR:O      | 9:CI:63:ILE:HG13  | 2.09                     | 0.52              |
| 16:CP:57:ARG:NH2   | 16:CP:79:VAL:O    | 2.40                     | 0.52              |
| 18:CR:82:THR:O     | 18:CR:83:GLU:HG2  | 2.09                     | 0.52              |
| 23:CW:20:A:H61     | 23:CW:46:U:H1'    | 1.70                     | 0.52              |
| 27:DA:2884:U:C2    | 54:D5:51:TYR:HE1  | 2.26                     | 0.52              |
| 55:D6:15:GLU:HB3   | 55:D6:18:ARG:HG2  | 1.91                     | 0.52              |
| 27:DA:2115:G:C4    | 27:DA:2117:A:N7   | 2.77                     | 0.52              |
| 27:DA:2313:C:H3'   | 27:DA:2313:C:H6   | 1.74                     | 0.52              |
| 27:DA:2466:C:O2'   | 27:DA:2467:C:H5'  | 2.09                     | 0.52              |
| 27:DA:2520:C:H2'   | 27:DA:2521:C:H6   | 1.73                     | 0.52              |
| 27:DA:31:C:H5''    | 27:DA:1239:G:OP1  | 2.09                     | 0.52              |
| 27:DA:45:C:OP2     | 27:DA:215:G:H2'   | 2.09                     | 0.52              |
| 27:DA:805:G:O2'    | 27:DA:806:C:OP1   | 2.22                     | 0.52              |
| 28:DB:95:C:H2'     | 28:DB:96:U:C6     | 2.44                     | 0.52              |
| 30:DD:211:ARG:HA   | 30:DD:214:TRP:CG  | 2.45                     | 0.52              |
| 32:DF:119:ARG:HG2  | 32:DF:119:ARG:O   | 2.10                     | 0.52              |
| 32:DF:83:PHE:O     | 32:DF:84:VAL:CB   | 2.57                     | 0.52              |
| 34:DH:64:LEU:O     | 34:DH:68:THR:HB   | 2.09                     | 0.52              |
| 34:DH:85:LYS:HG3   | 34:DH:145:ALA:HB2 | 1.90                     | 0.52              |
| 35:DI:58:LEU:C     | 35:DI:60:GLU:H    | 2.12                     | 0.52              |
| 42:DT:24:PRO:HA    | 42:DT:49:VAL:HG13 | 1.91                     | 0.52              |
| 44:DV:8:GLY:O      | 44:DV:10:LYS:HE2  | 2.10                     | 0.52              |
| 27:DA:496:G:H1'    | 45:DW:61:ASN:ND2  | 2.24                     | 0.52              |
| 47:DY:27:VAL:HA    | 47:DY:28:LYS:CE   | 2.39                     | 0.52              |
| 48:DZ:149:LEU:HD21 | 48:DZ:171:ALA:HB3 | 1.91                     | 0.52              |
| 1:AA:1058:G:H2'    | 1:AA:1059:C:C6    | 2.45                     | 0.52              |
| 1:AA:1494:G:N2     | 1:AA:1495:U:C2    | 2.78                     | 0.52              |
| 1:AA:176:C:O2'     | 1:AA:177:C:H5'    | 2.10                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:336:C:O2'    | 1:AA:337:C:H5'     | 2.09                     | 0.52              |
| 2:AB:162:ILE:HD11 | 2:AB:184:VAL:HG22  | 1.90                     | 0.52              |
| 2:AB:178:ARG:HH11 | 2:AB:178:ARG:HG2   | 1.74                     | 0.52              |
| 2:AB:54:THR:CB    | 2:AB:201:ILE:HD11  | 2.39                     | 0.52              |
| 4:AD:205:GLU:O    | 4:AD:207:TYR:N     | 2.43                     | 0.52              |
| 6:AF:10:LEU:HD13  | 6:AF:61:LEU:HD13   | 1.91                     | 0.52              |
| 8:AH:48:TYR:O     | 8:AH:49:GLU:CB     | 2.57                     | 0.52              |
| 10:AJ:52:GLY:O    | 14:AN:41:ARG:NH2   | 2.42                     | 0.52              |
| 1:AA:130:A:H5'    | 17:AQ:63:ARG:HE    | 1.75                     | 0.52              |
| 25:AY:6:U:H2'     | 25:AY:7:A:C8       | 2.44                     | 0.52              |
| 49:B0:24:LYS:HB2  | 49:B0:36:ILE:HD11  | 1.90                     | 0.52              |
| 51:B2:55:ARG:O    | 51:B2:58:ALA:N     | 2.41                     | 0.52              |
| 27:BA:1305:C:O2'  | 27:BA:1306:C:H5'   | 2.08                     | 0.52              |
| 27:BA:1332:G:N2   | 27:BA:1609:A:HO2'  | 2.06                     | 0.52              |
| 27:BA:2235:G:H2'  | 27:BA:2236:C:C6    | 2.45                     | 0.52              |
| 27:BA:2336:A:H61  | 49:B0:43:THR:CG2   | 2.21                     | 0.52              |
| 27:BA:2576:G:H3'  | 27:BA:2576:G:N3    | 2.24                     | 0.52              |
| 27:BA:574:C:N3    | 31:BE:145:LYS:NZ   | 2.53                     | 0.52              |
| 27:BA:644:A:C2'   | 27:BA:645:C:H5''   | 2.39                     | 0.52              |
| 27:BA:651:G:OP1   | 57:B8:19:SER:HB2   | 2.09                     | 0.52              |
| 27:BA:738:G:C6    | 27:BA:739:G:C2     | 2.98                     | 0.52              |
| 32:BF:70:THR:O    | 32:BF:72:ARG:N     | 2.42                     | 0.52              |
| 35:BI:11:ASN:HB3  | 35:BI:12:LEU:HD22  | 1.91                     | 0.52              |
| 35:BI:92:VAL:O    | 35:BI:92:VAL:HG22  | 2.09                     | 0.52              |
| 38:BP:17:LYS:HG3  | 38:BP:19:VAL:HG23  | 1.91                     | 0.52              |
| 40:BR:28:LEU:HD21 | 40:BR:114:VAL:HG12 | 1.91                     | 0.52              |
| 47:BY:67:LEU:HD13 | 47:BY:71:LYS:HE3   | 1.89                     | 0.52              |
| 1:CA:1158:C:O2    | 1:CA:1158:C:C2'    | 2.57                     | 0.52              |
| 1:CA:1343:G:H1'   | 9:CI:121:ARG:NH1   | 2.23                     | 0.52              |
| 1:CA:1419:G:H2'   | 1:CA:1420:C:C6     | 2.41                     | 0.52              |
| 1:CA:1423:G:O2'   | 1:CA:1424:C:H5'    | 2.09                     | 0.52              |
| 1:CA:607:A:C2'    | 1:CA:608:A:H5'     | 2.39                     | 0.52              |
| 1:CA:738:C:H5''   | 6:CF:69:GLU:HB2    | 1.91                     | 0.52              |
| 1:CA:955:U:H1'    | 1:CA:1227:A:N6     | 2.23                     | 0.52              |
| 2:CB:168:THR:HG23 | 2:CB:192:SER:CB    | 2.39                     | 0.52              |
| 3:CC:162:GLN:O    | 3:CC:164:ARG:HG3   | 2.09                     | 0.52              |
| 3:CC:39:ILE:C     | 3:CC:41:GLY:N      | 2.63                     | 0.52              |
| 6:CF:48:LEU:HD13  | 6:CF:52:ILE:CG1    | 2.39                     | 0.52              |
| 7:CG:15:ASP:O     | 7:CG:19:GLY:HA2    | 2.09                     | 0.52              |
| 9:CI:106:ALA:O    | 9:CI:108:VAL:N     | 2.42                     | 0.52              |
| 12:CL:123:LYS:C   | 12:CL:125:ALA:N    | 2.61                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:CL:5:ASN:HB2   | 17:CQ:34:LYS:HZ3  | 1.73                     | 0.52              |
| 14:CN:27:CYS:C    | 14:CN:29:ARG:N    | 2.61                     | 0.52              |
| 14:CN:44:LEU:O    | 14:CN:44:LEU:HD12 | 2.09                     | 0.52              |
| 15:CO:70:LEU:HD23 | 15:CO:78:TYR:HA   | 1.92                     | 0.52              |
| 17:CQ:17:LYS:HA   | 17:CQ:46:ASP:O    | 2.10                     | 0.52              |
| 20:CT:41:ILE:HA   | 20:CT:44:ALA:HB3  | 1.91                     | 0.52              |
| 51:D2:46:GLN:HA   | 51:D2:46:GLN:OE1  | 2.06                     | 0.52              |
| 55:D6:8:LYS:HG3   | 55:D6:8:LYS:O     | 2.09                     | 0.52              |
| 27:DA:1445:A:N3   | 27:DA:1445:A:H2'  | 2.24                     | 0.52              |
| 27:DA:1458:C:H5'  | 27:DA:1459:G:C8   | 2.44                     | 0.52              |
| 27:DA:1578:U:H2'  | 27:DA:1579:A:H5'' | 1.92                     | 0.52              |
| 27:DA:186:G:O2'   | 27:DA:187:G:H5'   | 2.10                     | 0.52              |
| 27:DA:2550:G:H2'  | 27:DA:2551:C:C5'  | 2.38                     | 0.52              |
| 27:DA:2757:A:N1   | 34:DH:67:LEU:HD22 | 2.25                     | 0.52              |
| 27:DA:301:G:C4    | 27:DA:302:C:C5    | 2.98                     | 0.52              |
| 27:DA:468:G:C6    | 27:DA:469:G:C4    | 2.97                     | 0.52              |
| 27:DA:819:A:H2'   | 27:DA:819:A:N3    | 2.24                     | 0.52              |
| 27:DA:923:C:H2'   | 27:DA:924:C:H6    | 1.74                     | 0.52              |
| 27:DA:998:C:H42   | 27:DA:1158:C:H42  | 1.57                     | 0.52              |
| 31:DE:37:ARG:O    | 31:DE:45:THR:HA   | 2.10                     | 0.52              |
| 31:DE:3:GLY:O     | 31:DE:4:ILE:CB    | 2.57                     | 0.52              |
| 33:DG:129:GLY:O   | 33:DG:161:THR:HB  | 2.08                     | 0.52              |
| 36:DN:25:ARG:NH1  | 36:DN:25:ARG:CG   | 2.71                     | 0.52              |
| 37:DO:13:ASN:C    | 37:DO:15:GLY:N    | 2.63                     | 0.52              |
| 41:DS:15:ARG:C    | 41:DS:17:ARG:O    | 2.48                     | 0.52              |
| 41:DS:97:ARG:HH22 | 41:DS:99:LYS:N    | 2.04                     | 0.52              |
| 42:DT:27:THR:O    | 42:DT:28:VAL:CB   | 2.57                     | 0.52              |
| 42:DT:25:GLY:O    | 42:DT:48:ILE:HG23 | 2.08                     | 0.52              |
| 42:DT:3:ARG:O     | 42:DT:7:ILE:HG12  | 2.10                     | 0.52              |
| 42:DT:50:ILE:HG23 | 42:DT:99:LEU:HD12 | 1.92                     | 0.52              |
| 44:DV:77:ALA:O    | 44:DV:79:VAL:N    | 2.42                     | 0.52              |
| 45:DW:21:VAL:CG1  | 45:DW:21:VAL:O    | 2.58                     | 0.52              |
| 45:DW:34:ASN:O    | 45:DW:37:ARG:HB3  | 2.10                     | 0.52              |
| 1:AA:1084:G:OP1   | 1:AA:1086:U:C4    | 2.63                     | 0.52              |
| 1:AA:1145:C:O2'   | 1:AA:1146:A:H5'   | 2.10                     | 0.52              |
| 1:AA:1416:G:N2    | 1:AA:1485:U:H1'   | 2.24                     | 0.52              |
| 1:AA:129(A):G:O2' | 1:AA:189(F):U:H2' | 2.09                     | 0.52              |
| 1:AA:506:G:C4     | 1:AA:507:C:C5     | 2.96                     | 0.52              |
| 1:AA:621:A:H2'    | 1:AA:622:A:H8     | 1.75                     | 0.52              |
| 2:AB:67:THR:OG1   | 2:AB:155:LEU:HD21 | 2.08                     | 0.52              |
| 11:AK:33:THR:HB   | 11:AK:37:GLY:O    | 2.10                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:AL:36:VAL:HG12 | 12:AL:38:ARG:H     | 1.74                     | 0.52              |
| 13:AM:116:THR:O   | 13:AM:117:VAL:HB   | 2.09                     | 0.52              |
| 13:AM:37:THR:OG1  | 13:AM:39:ILE:HD12  | 2.09                     | 0.52              |
| 15:AO:74:ASP:C    | 15:AO:76:GLU:N     | 2.62                     | 0.52              |
| 20:AT:89:ARG:NH1  | 20:AT:104:LEU:HD21 | 2.23                     | 0.52              |
| 20:AT:25:ARG:O    | 20:AT:28:ALA:HB3   | 2.10                     | 0.52              |
| 26:AZ:3:SER:O     | 26:AZ:5:UAL:N      | 2.38                     | 0.52              |
| 27:BA:2419:U:C5'  | 55:B6:23:THR:HG21  | 2.40                     | 0.52              |
| 57:B8:50:LEU:C    | 57:B8:53:PRO:HD2   | 2.28                     | 0.52              |
| 27:BA:1345:C:O2'  | 27:BA:1346:G:H5'   | 2.10                     | 0.52              |
| 27:BA:1578:U:H2'  | 27:BA:1578:U:O2    | 2.09                     | 0.52              |
| 27:BA:1578:U:H2'  | 27:BA:1579:A:C5'   | 2.38                     | 0.52              |
| 27:BA:1640:C:N4   | 27:BA:1641:A:C5    | 2.78                     | 0.52              |
| 27:BA:1945:G:C8   | 27:BA:1945:G:O5'   | 2.62                     | 0.52              |
| 27:BA:2241:A:C2   | 27:BA:2242:G:C5    | 2.98                     | 0.52              |
| 27:BA:352:G:C8    | 27:BA:355:G:O6     | 2.62                     | 0.52              |
| 27:BA:562:U:OP1   | 27:BA:562:U:H6     | 1.92                     | 0.52              |
| 27:BA:795:C:C6    | 27:BA:796:C:H5     | 2.27                     | 0.52              |
| 27:BA:988:A:H4'   | 27:BA:1155:A:C2    | 2.45                     | 0.52              |
| 27:BA:1820:U:O2   | 30:BD:201:HIS:HB3  | 2.10                     | 0.52              |
| 31:BE:63:LEU:O    | 31:BE:63:LEU:HD23  | 2.09                     | 0.52              |
| 32:BF:51:THR:HG23 | 32:BF:92:PRO:HG2   | 1.90                     | 0.52              |
| 34:BH:68:THR:C    | 34:BH:70:THR:N     | 2.61                     | 0.52              |
| 34:BH:87:LEU:HD22 | 34:BH:163:TYR:O    | 2.09                     | 0.52              |
| 40:BR:28:LEU:HA   | 40:BR:34:ILE:CG1   | 2.39                     | 0.52              |
| 42:BT:28:VAL:HG21 | 42:BT:46:GLU:CG    | 2.40                     | 0.52              |
| 46:BX:64:LYS:HE2  | 46:BX:73:ARG:HG3   | 1.92                     | 0.52              |
| 47:BY:50:ARG:CG   | 47:BY:58:GLY:HA3   | 2.38                     | 0.52              |
| 1:CA:119:A:O2'    | 1:CA:120:A:OP2     | 2.27                     | 0.52              |
| 1:CA:298:A:H8     | 1:CA:298:A:O5'     | 1.92                     | 0.52              |
| 1:CA:623:C:O2     | 1:CA:623:C:H2'     | 2.09                     | 0.52              |
| 1:CA:937:A:N6     | 1:CA:938:A:C6      | 2.77                     | 0.52              |
| 3:CC:76:VAL:HG23  | 3:CC:77:ILE:N      | 2.25                     | 0.52              |
| 4:CD:132:ARG:NH1  | 4:CD:132:ARG:HG2   | 2.24                     | 0.52              |
| 6:CF:12:PRO:HB3   | 6:CF:58:GLY:HA2    | 1.91                     | 0.52              |
| 7:CG:143:ARG:HH11 | 7:CG:143:ARG:CB    | 2.22                     | 0.52              |
| 1:CA:1347:G:C8    | 9:CI:107:ARG:HB3   | 2.45                     | 0.52              |
| 12:CL:25:LYS:HZ1  | 12:CL:30:ARG:HH22  | 1.55                     | 0.52              |
| 17:CQ:45:HIS:CD2  | 17:CQ:47:PRO:HD3   | 2.45                     | 0.52              |
| 49:D0:40:GLN:HE22 | 49:D0:45:PHE:H     | 1.56                     | 0.52              |
| 52:D3:12:PRO:O    | 52:D3:20:LYS:NZ    | 2.42                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 54:D5:49:CYS:O     | 54:D5:56:LYS:HB2  | 2.09                     | 0.52              |
| 55:D6:8:LYS:O      | 55:D6:9:LEU:CB    | 2.57                     | 0.52              |
| 27:DA:1455:G:O2'   | 27:DA:1456:G:H5'  | 2.09                     | 0.52              |
| 27:DA:1884:A:N1    | 27:DA:1885:A:C5   | 2.78                     | 0.52              |
| 27:DA:1899:G:N2    | 27:DA:1903:G:C2   | 2.77                     | 0.52              |
| 27:DA:18:C:C4      | 27:DA:19:C:C5     | 2.98                     | 0.52              |
| 27:DA:2010:G:C6    | 27:DA:2011:U:C4   | 2.97                     | 0.52              |
| 27:DA:2356:C:H4'   | 49:D0:20:ARG:HD3  | 1.90                     | 0.52              |
| 27:DA:2489:G:H2'   | 27:DA:2490:G:O4'  | 2.10                     | 0.52              |
| 27:DA:2580:U:H4'   | 31:DE:130:GLY:CA  | 2.40                     | 0.52              |
| 27:DA:272(D):G:C2  | 27:DA:365:C:C4    | 2.98                     | 0.52              |
| 27:DA:2749:A:H4'   | 34:DH:62:LYS:CB   | 2.29                     | 0.52              |
| 27:DA:660:G:O2'    | 27:DA:661:C:H5'   | 2.10                     | 0.52              |
| 27:DA:999:U:O2     | 27:DA:1000:A:H8   | 1.92                     | 0.52              |
| 28:DB:4:C:H2'      | 28:DB:5:C:C6      | 2.45                     | 0.52              |
| 27:DA:574:C:N3     | 31:DE:145:LYS:HE2 | 2.24                     | 0.52              |
| 27:DA:1248:G:OP1   | 32:DF:92:PRO:HB3  | 2.08                     | 0.52              |
| 33:DG:110:ALA:O    | 33:DG:111:LEU:C   | 2.47                     | 0.52              |
| 42:DT:21:GLU:HG3   | 42:DT:22:PHE:N    | 2.25                     | 0.52              |
| 44:DV:21:ARG:HG2   | 44:DV:91:TYR:CE1  | 2.44                     | 0.52              |
| 47:DY:15:VAL:HG12  | 47:DY:16:ALA:H    | 1.73                     | 0.52              |
| 47:DY:4:LYS:HG3    | 47:DY:5:MET:HE3   | 1.91                     | 0.52              |
| 47:DY:76:CYS:O     | 47:DY:78:ALA:N    | 2.42                     | 0.52              |
| 1:AA:1179:A:C5'    | 9:AI:102:LEU:HD12 | 2.39                     | 0.52              |
| 1:AA:1236:A:H4'    | 1:AA:1304:G:H4'   | 1.92                     | 0.52              |
| 1:AA:1271:G:H5'    | 1:AA:1314:C:H5'   | 1.92                     | 0.52              |
| 1:AA:1338:G:H2'    | 1:AA:1339:A:O4'   | 2.10                     | 0.52              |
| 1:AA:1426:C:H2'    | 1:AA:1427:U:H6    | 1.75                     | 0.52              |
| 1:AA:939:G:H2'     | 1:AA:940:C:C6     | 2.45                     | 0.52              |
| 3:AC:150:LYS:CG    | 3:AC:169:ALA:HB2  | 2.38                     | 0.52              |
| 7:AG:103:TRP:CE3   | 7:AG:137:LYS:HB3  | 2.45                     | 0.52              |
| 7:AG:15:ASP:OD2    | 7:AG:16:LEU:N     | 2.42                     | 0.52              |
| 15:AO:56:LEU:O     | 15:AO:60:VAL:HG23 | 2.10                     | 0.52              |
| 19:AS:12:ASP:HB3   | 19:AS:14:HIS:CE1  | 2.45                     | 0.52              |
| 19:AS:61:TYR:O     | 19:AS:62:ILE:HG22 | 2.10                     | 0.52              |
| 20:AT:73:HIS:O     | 20:AT:76:ALA:HB3  | 2.09                     | 0.52              |
| 50:B1:18:ILE:HG21  | 50:B1:20:ARG:CZ   | 2.39                     | 0.52              |
| 50:B1:20:ARG:O     | 50:B1:21:ARG:HG2  | 2.09                     | 0.52              |
| 51:B2:17:SER:H     | 51:B2:67:LYS:HZ1  | 1.57                     | 0.52              |
| 33:BG:109:VAL:HG13 | 53:B4:59:VAL:HG11 | 1.90                     | 0.52              |
| 27:BA:1261:C:H2'   | 27:BA:1262:A:O5'  | 2.09                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1578:U:H2'  | 27:BA:1579:A:H5'   | 1.90                     | 0.52              |
| 27:BA:1686:C:C6   | 27:BA:1686:C:C5'   | 2.89                     | 0.52              |
| 27:BA:1799:G:H5'' | 27:BA:1802:A:O2'   | 2.09                     | 0.52              |
| 27:BA:2285:C:H41  | 55:B6:25:LYS:HE3   | 1.75                     | 0.52              |
| 27:BA:2693:A:C2'  | 27:BA:2694:G:H5'   | 2.38                     | 0.52              |
| 27:BA:307:G:H8    | 27:BA:307:G:O5'    | 1.92                     | 0.52              |
| 27:BA:344:G:N2    | 27:BA:345:A:N6     | 2.54                     | 0.52              |
| 27:BA:481:G:OP2   | 47:BY:47:LYS:HG3   | 2.09                     | 0.52              |
| 32:BF:127:GLU:OE1 | 32:BF:196:LEU:HG   | 2.10                     | 0.52              |
| 32:BF:160:ASN:ND2 | 32:BF:160:ASN:C    | 2.62                     | 0.52              |
| 27:BA:444:C:C4'   | 32:BF:49:ALA:HB2   | 2.39                     | 0.52              |
| 33:BG:170:ARG:NH2 | 33:BG:182:LYS:HG3  | 2.25                     | 0.52              |
| 37:BO:1:MET:C     | 37:BO:2:ILE:HD13   | 2.29                     | 0.52              |
| 39:BQ:36:ALA:O    | 39:BQ:37:LEU:HD22  | 2.09                     | 0.52              |
| 40:BR:52:ILE:O    | 40:BR:55:ALA:N     | 2.43                     | 0.52              |
| 42:BT:109:GLU:HA  | 42:BT:112:ARG:HD3  | 1.91                     | 0.52              |
| 44:BV:15:GLU:O    | 44:BV:16:PRO:C     | 2.48                     | 0.52              |
| 47:BY:47:LYS:O    | 47:BY:48:ALA:O     | 2.26                     | 0.52              |
| 47:BY:3:VAL:C     | 47:BY:5:MET:N      | 2.60                     | 0.52              |
| 1:CA:1305:G:O2'   | 1:CA:1306:A:P      | 2.68                     | 0.52              |
| 1:CA:186:C:H2'    | 1:CA:187:C:C5      | 2.45                     | 0.52              |
| 1:CA:252:U:H2'    | 1:CA:253:U:C6      | 2.45                     | 0.52              |
| 1:CA:255:G:H2'    | 1:CA:256:U:C6      | 2.45                     | 0.52              |
| 1:CA:678:U:O2     | 1:CA:777:A:H4'     | 2.09                     | 0.52              |
| 2:CB:43:ASP:OD2   | 2:CB:46:LYS:HB2    | 2.10                     | 0.52              |
| 4:CD:179:GLU:O    | 4:CD:181:MET:HG3   | 2.09                     | 0.52              |
| 1:CA:963:G:H21    | 10:CJ:55:LYS:CD    | 2.21                     | 0.52              |
| 17:CQ:27:PHE:HB2  | 17:CQ:28:PRO:CD    | 2.40                     | 0.52              |
| 20:CT:45:GLN:C    | 20:CT:47:GLY:H     | 2.12                     | 0.52              |
| 27:DA:747:U:N3    | 54:D5:2:ALA:N      | 2.58                     | 0.52              |
| 58:D9:10:ILE:HD12 | 58:D9:32:HIS:CD2   | 2.44                     | 0.52              |
| 27:DA:1188:U:C2'  | 27:DA:1189:A:H5'   | 2.40                     | 0.52              |
| 27:DA:1473:G:H2'  | 27:DA:1474:C:C5'   | 2.37                     | 0.52              |
| 27:DA:154(A):C:O2 | 27:DA:154(A):C:O4' | 2.26                     | 0.52              |
| 27:DA:2351:G:H5'' | 27:DA:2352:A:OP1   | 2.08                     | 0.52              |
| 27:DA:2405:G:O2'  | 27:DA:2406:U:P     | 2.67                     | 0.52              |
| 27:DA:2529:G:OP2  | 27:DA:2530:A:H5''  | 2.09                     | 0.52              |
| 27:DA:25:U:H2'    | 27:DA:26:G:O4'     | 2.09                     | 0.52              |
| 27:DA:2680:C:OP2  | 31:DE:111:ARG:NH2  | 2.43                     | 0.52              |
| 27:DA:2889:C:H3'  | 27:DA:2891:G:C8    | 2.44                     | 0.52              |
| 27:DA:492:A:C8    | 27:DA:493:G:C8     | 2.98                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:DA:774:A:H2   | 27:DA:787:U:O2'   | 1.90                     | 0.52              |
| 29:DC:68:LEU:CD1 | 29:DC:179:SER:HA  | 2.40                     | 0.52              |
| 27:DA:2729:G:O3' | 31:DE:185:LYS:NZ  | 2.43                     | 0.52              |
| 31:DE:1:MET:H3   | 31:DE:84:PHE:HB2  | 1.75                     | 0.52              |
| 32:DF:31:HIS:CD2 | 32:DF:35:GLU:HG3  | 2.45                     | 0.52              |
| 39:DQ:10:ARG:HG3 | 39:DQ:10:ARG:O    | 2.09                     | 0.52              |
| 39:DQ:132:VAL:HB | 39:DQ:137:TYR:OH  | 2.09                     | 0.52              |
| 39:DQ:35:VAL:HA  | 39:DQ:102:VAL:HA  | 1.90                     | 0.52              |
| 39:DQ:45:GLN:NE2 | 39:DQ:45:GLN:N    | 2.49                     | 0.52              |
| 40:DR:14:SER:OG  | 40:DR:15:SER:N    | 2.40                     | 0.52              |
| 40:DR:41:ALA:C   | 40:DR:43:GLU:N    | 2.62                     | 0.52              |
| 42:DT:32:TYR:CD2 | 42:DT:32:TYR:N    | 2.76                     | 0.52              |
| 42:DT:55:ASN:O   | 42:DT:55:ASN:ND2  | 2.32                     | 0.52              |
| 27:DA:29:U:H4'   | 43:DU:11:ARG:HH22 | 1.72                     | 0.52              |
| 43:DU:81:HIS:O   | 43:DU:85:LYS:HB2  | 2.09                     | 0.52              |
| 47:DY:18:GLY:C   | 47:DY:20:TYR:H    | 2.13                     | 0.52              |
| 1:AA:1054:C:C6   | 1:AA:1196:U:H2'   | 2.45                     | 0.52              |
| 1:AA:1346:A:C5'  | 9:AI:120:ARG:HH12 | 2.23                     | 0.52              |
| 1:AA:1372:U:OP2  | 9:AI:11:LYS:HE3   | 2.09                     | 0.52              |
| 1:AA:604:G:C6    | 1:AA:635:G:C6     | 2.98                     | 0.52              |
| 1:AA:909:A:O2'   | 1:AA:910:C:H5'    | 2.08                     | 0.52              |
| 2:AB:15:VAL:C    | 2:AB:16:HIS:CG    | 2.83                     | 0.52              |
| 4:AD:64:LEU:HB2  | 4:AD:198:VAL:CG1  | 2.40                     | 0.52              |
| 5:AE:99:GLY:O    | 5:AE:116:THR:O    | 2.27                     | 0.52              |
| 6:AF:10:LEU:CD1  | 6:AF:61:LEU:HD13  | 2.39                     | 0.52              |
| 9:AI:15:ALA:HB2  | 9:AI:65:VAL:HG23  | 1.91                     | 0.52              |
| 10:AJ:25:GLU:C   | 10:AJ:27:ALA:H    | 2.11                     | 0.52              |
| 9:AI:114:TYR:HE1 | 10:AJ:60:ARG:N    | 2.08                     | 0.52              |
| 25:AY:62:U:H2'   | 25:AY:63:C:O4'    | 2.10                     | 0.52              |
| 55:B6:29:ASN:ND2 | 55:B6:30:THR:H    | 2.07                     | 0.52              |
| 27:BA:1015:G:H8  | 27:BA:1015:G:H5'' | 1.73                     | 0.52              |
| 27:BA:1176:G:O2' | 27:BA:1177:A:H5'  | 2.10                     | 0.52              |
| 27:BA:1199:U:H2' | 27:BA:1200:C:H6   | 1.74                     | 0.52              |
| 27:BA:1291:C:C2  | 27:BA:1292:U:C5   | 2.98                     | 0.52              |
| 27:BA:1627:G:N3  | 27:BA:1628:G:C8   | 2.78                     | 0.52              |
| 27:BA:1710:C:C6  | 27:BA:1710:C:H3'  | 2.45                     | 0.52              |
| 27:BA:1778:U:H2' | 27:BA:1784:A:N6   | 2.24                     | 0.52              |
| 27:BA:2290:G:C2  | 27:BA:2343:C:O2   | 2.63                     | 0.52              |
| 27:BA:2308:G:C2' | 27:BA:2309:A:O5'  | 2.58                     | 0.52              |
| 27:BA:2578:G:H2' | 27:BA:2579:C:C6   | 2.44                     | 0.52              |
| 27:BA:2606:C:O2' | 27:BA:2607:G:H5'  | 2.10                     | 0.52              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 27:BA:2801(A):A:C4' | 27:BA:2802:G:H5'  | 2.21                     | 0.52              |
| 27:BA:372:G:O2'     | 27:BA:373:U:P     | 2.67                     | 0.52              |
| 29:BC:72:VAL:HG21   | 29:BC:161:ILE:CA  | 2.40                     | 0.52              |
| 30:BD:12:SER:C      | 30:BD:14:ARG:H    | 2.13                     | 0.52              |
| 30:BD:254:THR:O     | 30:BD:254:THR:OG1 | 2.23                     | 0.52              |
| 33:BG:31:VAL:HG22   | 33:BG:32:PRO:HD2  | 1.91                     | 0.52              |
| 34:BH:44:VAL:O      | 34:BH:46:GLU:CD   | 2.48                     | 0.52              |
| 37:BO:60:ALA:HB2    | 37:BO:86:ILE:HA   | 1.92                     | 0.52              |
| 37:BO:90:GLN:O      | 37:BO:91:LEU:HB2  | 2.09                     | 0.52              |
| 38:BP:144:GLU:O     | 38:BP:145:PRO:C   | 2.48                     | 0.52              |
| 38:BP:91:PHE:HZ     | 38:BP:100:LEU:CD1 | 2.23                     | 0.52              |
| 41:BS:92:TYR:CG     | 41:BS:93:LYS:N    | 2.78                     | 0.52              |
| 42:BT:16:ARG:HH11   | 42:BT:19:LEU:HD11 | 1.74                     | 0.52              |
| 45:BW:15:ARG:O      | 45:BW:18:ARG:HB2  | 2.09                     | 0.52              |
| 1:CA:1285:A:H4'     | 1:CA:1286:A:O5'   | 2.09                     | 0.52              |
| 1:CA:1466:C:H2'     | 1:CA:1467:G:O4'   | 2.10                     | 0.52              |
| 1:CA:748:C:O2'      | 1:CA:749:C:OP2    | 2.25                     | 0.52              |
| 1:CA:882:C:N4       | 12:CL:2:PRO:HG3   | 2.24                     | 0.52              |
| 1:CA:5:U:C2'        | 4:CD:86:LYS:HE2   | 2.39                     | 0.52              |
| 5:CE:102:ALA:HB2    | 5:CE:120:THR:OG1  | 2.09                     | 0.52              |
| 7:CG:135:VAL:O      | 7:CG:138:LYS:HB3  | 2.09                     | 0.52              |
| 8:CH:7:ALA:CB       | 8:CH:85:ARG:HG3   | 2.39                     | 0.52              |
| 14:CN:26:ARG:HH22   | 14:CN:47:LEU:HD21 | 1.74                     | 0.52              |
| 19:CS:22:LEU:N      | 19:CS:22:LEU:CD2  | 2.72                     | 0.52              |
| 49:D0:30:VAL:HG12   | 49:D0:66:VAL:HG22 | 1.92                     | 0.52              |
| 51:D2:52:ASP:O      | 51:D2:55:ARG:N    | 2.43                     | 0.52              |
| 57:D8:10:ALA:CB     | 57:D8:60:LEU:HD21 | 2.34                     | 0.52              |
| 58:D9:7:VAL:HG13    | 58:D9:34:GLN:OE1  | 2.10                     | 0.52              |
| 27:DA:1013:C:N4     | 27:DA:1149:G:H1   | 2.07                     | 0.52              |
| 27:DA:1280:G:N2     | 27:DA:1281:G:H1'  | 2.24                     | 0.52              |
| 27:DA:1683:C:H42    | 27:DA:1705:G:H1   | 1.58                     | 0.52              |
| 27:DA:171:G:H2'     | 27:DA:172:C:C6    | 2.44                     | 0.52              |
| 27:DA:1810:A:C8     | 27:DA:1811:G:C8   | 2.98                     | 0.52              |
| 27:DA:211:A:O2'     | 27:DA:212:G:H5'   | 2.10                     | 0.52              |
| 27:DA:2188:C:H2'    | 27:DA:2189:U:O4'  | 2.08                     | 0.52              |
| 27:DA:2809:A:OP2    | 27:DA:2891:G:N2   | 2.40                     | 0.52              |
| 27:DA:2824:C:N4     | 27:DA:2825:C:N3   | 2.57                     | 0.52              |
| 27:DA:587:C:C6      | 38:DP:33:ARG:CZ   | 2.92                     | 0.52              |
| 27:DA:67:U:C2       | 27:DA:68:G:C8     | 2.97                     | 0.52              |
| 27:DA:58:G:O2'      | 27:DA:73:A:N1     | 2.35                     | 0.52              |
| 28:DB:53:A:H2'      | 28:DB:53:A:N3     | 2.24                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2126:A:H5''  | 29:DC:36:LYS:HG2   | 1.90                     | 0.52              |
| 30:DD:46:GLN:N     | 30:DD:46:GLN:OE1   | 2.43                     | 0.52              |
| 31:DE:93:VAL:HG11  | 31:DE:181:LEU:O    | 2.09                     | 0.52              |
| 32:DF:202:PHE:O    | 32:DF:204:ASN:N    | 2.43                     | 0.52              |
| 32:DF:2:LYS:O      | 32:DF:25:PRO:CD    | 2.55                     | 0.52              |
| 33:DG:128:ARG:C    | 33:DG:130:ASN:N    | 2.63                     | 0.52              |
| 34:DH:143:GLN:NE2  | 34:DH:147:ASN:OD1  | 2.43                     | 0.52              |
| 35:DI:12:LEU:HB2   | 35:DI:19:VAL:HG21  | 1.92                     | 0.52              |
| 38:DP:138:LEU:HG   | 38:DP:142:GLY:HA3  | 1.92                     | 0.52              |
| 40:DR:26:LYS:HZ3   | 40:DR:71:GLN:HB3   | 1.74                     | 0.52              |
| 27:DA:1252:G:N2    | 43:DU:33:ARG:HD2   | 2.24                     | 0.52              |
| 43:DU:57:PHE:O     | 43:DU:58:ARG:C     | 2.47                     | 0.52              |
| 27:DA:495:G:H21    | 45:DW:61:ASN:HD21  | 1.57                     | 0.52              |
| 46:DX:26:TYR:CE2   | 46:DX:89:ILE:HB    | 2.43                     | 0.52              |
| 1:AA:1158:C:C2'    | 1:AA:1158:C:O2     | 2.54                     | 0.52              |
| 1:AA:1186:G:N2     | 1:AA:1187:G:H1'    | 2.23                     | 0.52              |
| 1:AA:1214:C:C6     | 1:AA:1214:C:OP1    | 2.63                     | 0.52              |
| 1:AA:885:G:O2'     | 1:AA:886:G:H5'     | 2.09                     | 0.52              |
| 1:AA:986:A:H2'     | 1:AA:987:G:C8      | 2.45                     | 0.52              |
| 2:AB:155:LEU:HD13  | 2:AB:157:ARG:H     | 1.74                     | 0.52              |
| 3:AC:50:ALA:O      | 3:AC:51:GLY:O      | 2.27                     | 0.52              |
| 1:AA:1298:C:C5     | 7:AG:114:ARG:HD2   | 2.45                     | 0.52              |
| 7:AG:58:PRO:O      | 7:AG:61:VAL:HB     | 2.08                     | 0.52              |
| 10:AJ:96:ILE:CD1   | 10:AJ:96:ILE:N     | 2.68                     | 0.52              |
| 13:AM:65:LYS:CG    | 13:AM:70:LEU:HB2   | 2.40                     | 0.52              |
| 17:AQ:45:HIS:N     | 17:AQ:69:LYS:HE2   | 2.25                     | 0.52              |
| 25:AY:71:A:H2'     | 25:AY:72:G:O4'     | 2.10                     | 0.52              |
| 27:BA:1292:U:C2    | 27:BA:1293:C:C5    | 2.98                     | 0.52              |
| 27:BA:1337:G:H2'   | 27:BA:1338:G:C8    | 2.43                     | 0.52              |
| 27:BA:1451:C:HO2'  | 27:BA:1457:A:N6    | 2.08                     | 0.52              |
| 27:BA:1504:C:C2'   | 27:BA:1505:C:H5''  | 2.40                     | 0.52              |
| 27:BA:1776:G:C6    | 27:BA:1777:U:C4    | 2.98                     | 0.52              |
| 27:BA:1835:G:C5'   | 27:BA:1836:C:OP2   | 2.56                     | 0.52              |
| 27:BA:1884:A:H2'   | 27:BA:1885:A:C5'   | 2.25                     | 0.52              |
| 27:BA:2594:C:H2'   | 27:BA:2595:G:C8    | 2.45                     | 0.52              |
| 27:BA:2767:C:H2'   | 27:BA:2768:C:C6    | 2.44                     | 0.52              |
| 27:BA:352:G:H8     | 27:BA:355:G:O6     | 1.93                     | 0.52              |
| 31:BE:69:LYS:HZ1   | 31:BE:89:ASP:HA    | 1.74                     | 0.52              |
| 32:BF:186:ILE:HD13 | 32:BF:192:LEU:HD12 | 1.92                     | 0.52              |
| 32:BF:3:GLU:HB3    | 32:BF:20:LEU:O     | 2.10                     | 0.52              |
| 37:BO:35:VAL:HG23  | 37:BO:65:THR:CG2   | 2.40                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BP:17:LYS:C     | 38:BP:19:VAL:H     | 2.11                     | 0.52              |
| 39:BQ:17:LEU:N     | 39:BQ:17:LEU:HD23  | 2.25                     | 0.52              |
| 39:BQ:26:TYR:O     | 39:BQ:67:ARG:NH1   | 2.43                     | 0.52              |
| 39:BQ:46:GLN:O     | 39:BQ:49:ALA:N     | 2.43                     | 0.52              |
| 39:BQ:63:LYS:HD3   | 39:BQ:65:PHE:CZ    | 2.45                     | 0.52              |
| 40:BR:33:ARG:HA    | 40:BR:114:VAL:O    | 2.10                     | 0.52              |
| 43:BU:24:TYR:CE1   | 43:BU:38:THR:CG2   | 2.93                     | 0.52              |
| 44:BV:35:LEU:HD23  | 44:BV:35:LEU:N     | 2.24                     | 0.52              |
| 48:BZ:13:LYS:O     | 48:BZ:17:LEU:HD13  | 2.10                     | 0.52              |
| 1:CA:1064:G:HO2'   | 1:CA:1065:U:C5'    | 2.22                     | 0.52              |
| 1:CA:1196:U:OP1    | 1:CA:1197:G:H5'    | 2.10                     | 0.52              |
| 1:CA:1437:C:H2'    | 1:CA:1438:G:H8     | 1.74                     | 0.52              |
| 1:CA:255:G:H2'     | 1:CA:256:U:H6      | 1.74                     | 0.52              |
| 1:CA:341:C:O2'     | 1:CA:342:C:H5'     | 2.09                     | 0.52              |
| 1:CA:461:A:N7      | 1:CA:471:G:N7      | 2.58                     | 0.52              |
| 1:CA:487:A:H2'     | 1:CA:488:C:O4'     | 2.09                     | 0.52              |
| 1:CA:505:G:H2'     | 1:CA:506:G:H8      | 1.73                     | 0.52              |
| 2:CB:70:PHE:O      | 2:CB:92:TYR:HA     | 2.10                     | 0.52              |
| 3:CC:22:TRP:HH2    | 3:CC:32:LEU:O      | 1.93                     | 0.52              |
| 4:CD:60:GLU:O      | 4:CD:63:LYS:HB2    | 2.10                     | 0.52              |
| 4:CD:93:PHE:CE1    | 4:CD:97:LEU:HD11   | 2.44                     | 0.52              |
| 9:CI:22:GLY:HA3    | 9:CI:60:ASP:OD2    | 2.09                     | 0.52              |
| 1:CA:691:G:O6      | 11:CK:55:LYS:HE2   | 2.10                     | 0.52              |
| 12:CL:48:ALA:C     | 12:CL:49:LEU:HD22  | 2.30                     | 0.52              |
| 1:CA:1321:C:C4'    | 13:CM:87:TYR:CE2   | 2.92                     | 0.52              |
| 17:CQ:57:VAL:CG1   | 17:CQ:76:LEU:HA    | 2.32                     | 0.52              |
| 20:CT:13:LEU:O     | 20:CT:16:HIS:HB3   | 2.09                     | 0.52              |
| 50:D1:23:LYS:HE2   | 50:D1:28:GLY:HA3   | 1.91                     | 0.52              |
| 27:DA:1011:G:C2    | 27:DA:1013:C:C2    | 2.97                     | 0.52              |
| 27:DA:1173:G:H3'   | 27:DA:1174:A:H5'   | 1.92                     | 0.52              |
| 27:DA:1174:A:H5''  | 27:DA:1175:U:C5'   | 2.40                     | 0.52              |
| 27:DA:1271:G:C2    | 27:DA:1617:C:H4'   | 2.45                     | 0.52              |
| 27:DA:1291:C:O2'   | 27:DA:1292:U:H5'   | 2.09                     | 0.52              |
| 27:DA:142:A:H8     | 27:DA:1408:C:H1'   | 1.69                     | 0.52              |
| 27:DA:2066:C:OP1   | 27:DA:2252:G:H4'   | 2.09                     | 0.52              |
| 27:DA:2271:G:H2'   | 27:DA:2272:U:H6    | 1.75                     | 0.52              |
| 27:DA:2317:C:O2'   | 27:DA:2318:G:H5'   | 2.10                     | 0.52              |
| 27:DA:271(S):G:C2' | 27:DA:271(T):C:C5' | 2.80                     | 0.52              |
| 27:DA:2756:U:O2'   | 27:DA:2757:A:C5'   | 2.56                     | 0.52              |
| 27:DA:419:C:O2'    | 27:DA:420:C:H5'    | 2.10                     | 0.52              |
| 27:DA:602:G:O2'    | 27:DA:604:G:H4'    | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:673:C:OP1   | 32:DF:54:ARG:NH1  | 2.43                     | 0.52              |
| 27:DA:743:G:O2'   | 27:DA:744:G:H5'   | 2.10                     | 0.52              |
| 27:DA:845:G:H8    | 27:DA:845:G:C5'   | 2.23                     | 0.52              |
| 27:DA:943:U:OP2   | 38:DP:38:GLN:CD   | 2.48                     | 0.52              |
| 30:DD:26:LYS:NZ   | 30:DD:82:ILE:H    | 2.07                     | 0.52              |
| 31:DE:30:PRO:HD3  | 31:DE:180:ASN:OD1 | 2.09                     | 0.52              |
| 32:DF:54:ARG:NH2  | 32:DF:80:ALA:HB2  | 2.24                     | 0.52              |
| 33:DG:66:GLN:HB3  | 33:DG:92:VAL:HG21 | 1.91                     | 0.52              |
| 36:DN:75:TYR:HA   | 36:DN:81:GLY:O    | 2.10                     | 0.52              |
| 40:DR:33:ARG:HG3  | 40:DR:115:GLU:CB  | 2.40                     | 0.52              |
| 40:DR:37:THR:OG1  | 40:DR:40:LYS:HE3  | 2.09                     | 0.52              |
| 40:DR:99:LYS:HB2  | 40:DR:99:LYS:NZ   | 2.25                     | 0.52              |
| 44:DV:47:VAL:HG12 | 44:DV:52:VAL:CB   | 2.38                     | 0.52              |
| 46:DX:36:LYS:CE   | 46:DX:56:THR:H    | 2.23                     | 0.52              |
| 46:DX:54:VAL:HG22 | 46:DX:81:VAL:HG12 | 1.90                     | 0.52              |
| 47:DY:2:ARG:O     | 47:DY:3:VAL:HG23  | 2.10                     | 0.52              |
| 1:AA:1002:G:N2    | 1:AA:1039:C:O2    | 2.43                     | 0.52              |
| 1:AA:120:A:HO2'   | 1:AA:121:C:P      | 2.32                     | 0.52              |
| 1:AA:194:C:C2'    | 1:AA:195:A:H5''   | 2.39                     | 0.52              |
| 1:AA:503:C:OP1    | 12:AL:116:LYS:HE3 | 2.10                     | 0.52              |
| 1:AA:581:G:O5'    | 1:AA:581:G:H8     | 1.93                     | 0.52              |
| 5:AE:129:ILE:O    | 5:AE:132:ALA:N    | 2.24                     | 0.52              |
| 1:AA:1298:C:N4    | 7:AG:114:ARG:HD2  | 2.25                     | 0.52              |
| 7:AG:41:ARG:HG2   | 7:AG:41:ARG:NH1   | 2.25                     | 0.52              |
| 10:AJ:32:ALA:H    | 10:AJ:76:ASN:HB3  | 1.74                     | 0.52              |
| 13:AM:65:LYS:HB3  | 13:AM:70:LEU:HD12 | 1.91                     | 0.52              |
| 17:AQ:79:SER:OG   | 17:AQ:80:GLY:N    | 2.41                     | 0.52              |
| 18:AR:86:VAL:HG12 | 18:AR:87:ARG:HD3  | 1.91                     | 0.52              |
| 1:AA:1320:C:N4    | 19:AS:36:ARG:HG3  | 2.24                     | 0.52              |
| 1:AA:194:C:O2'    | 20:AT:68:LYS:HD3  | 2.08                     | 0.52              |
| 50:B1:57:GLU:O    | 50:B1:58:ILE:HG23 | 2.09                     | 0.52              |
| 51:B2:24:LEU:HD11 | 51:B2:28:LYS:HE2  | 1.92                     | 0.52              |
| 27:BA:1108:U:C2'  | 27:BA:1109:C:H5'  | 2.40                     | 0.52              |
| 27:BA:1140:C:O3'  | 36:BN:25:ARG:NH1  | 2.43                     | 0.52              |
| 27:BA:1545:A:H3'  | 27:BA:1546:C:H6   | 1.75                     | 0.52              |
| 27:BA:1711:C:H2'  | 27:BA:1712:C:H6   | 1.75                     | 0.52              |
| 27:BA:1899:G:H21  | 27:BA:1902:C:H5   | 1.58                     | 0.52              |
| 27:BA:2839:G:H2'  | 27:BA:2840:C:C6   | 2.43                     | 0.52              |
| 27:BA:445:C:N4    | 27:BA:446:G:C6    | 2.78                     | 0.52              |
| 27:BA:775:G:C2    | 27:BA:777:A:N6    | 2.78                     | 0.52              |
| 27:BA:816:C:H2'   | 27:BA:817:C:C6    | 2.44                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BD:27:THR:CG2  | 30:BD:83:GLU:HA    | 2.40                     | 0.52              |
| 31:BE:26:ILE:HG22 | 31:BE:27:LEU:N     | 2.25                     | 0.52              |
| 33:BG:53:LEU:N    | 33:BG:53:LEU:CD2   | 2.73                     | 0.52              |
| 35:BI:89:TYR:C    | 35:BI:121:LYS:NZ   | 2.63                     | 0.52              |
| 27:BA:941:A:O2'   | 38:BP:35:HIS:CE1   | 2.63                     | 0.52              |
| 38:BP:38:GLN:HG3  | 38:BP:39:LYS:H     | 1.75                     | 0.52              |
| 41:BS:87:PHE:HZ   | 41:BS:97:ARG:HH22  | 1.57                     | 0.52              |
| 41:BS:92:TYR:N    | 41:BS:92:TYR:CD1   | 2.78                     | 0.52              |
| 44:BV:95:LEU:HD22 | 44:BV:96:ILE:N     | 2.25                     | 0.52              |
| 47:BY:53:PRO:HB3  | 47:BY:56:PRO:HA    | 1.91                     | 0.52              |
| 1:CA:1054:C:C5    | 1:CA:1196:U:C6     | 2.98                     | 0.52              |
| 1:CA:12:U:O2'     | 1:CA:13:U:H5''     | 2.09                     | 0.52              |
| 1:CA:392:G:H2'    | 1:CA:393:A:H8      | 1.75                     | 0.52              |
| 2:CB:174:VAL:HG13 | 2:CB:184:VAL:CG2   | 2.38                     | 0.52              |
| 4:CD:133:VAL:HG11 | 4:CD:138:TYR:CD1   | 2.44                     | 0.52              |
| 7:CG:66:VAL:HG12  | 7:CG:67:GLU:N      | 2.24                     | 0.52              |
| 8:CH:29:SER:O     | 8:CH:32:LYS:N      | 2.41                     | 0.52              |
| 14:CN:35:ARG:HH11 | 14:CN:35:ARG:HG2   | 1.74                     | 0.52              |
| 1:CA:624:C:H4'    | 16:CP:10:GLY:C     | 2.29                     | 0.52              |
| 20:CT:50:GLU:HA   | 20:CT:100:ILE:HG21 | 1.92                     | 0.52              |
| 52:D3:8:LEU:HB3   | 52:D3:31:LEU:HD23  | 1.91                     | 0.52              |
| 52:D3:39:ASP:OD2  | 52:D3:44:ARG:NH2   | 2.42                     | 0.52              |
| 53:D4:61:VAL:HG13 | 53:D4:65:CYS:CB    | 2.39                     | 0.52              |
| 54:D5:42:PRO:O    | 54:D5:43:HIS:CB    | 2.58                     | 0.52              |
| 27:DA:1114:G:H3'  | 27:DA:1115:G:H5''  | 1.92                     | 0.52              |
| 27:DA:171:G:O2'   | 27:DA:172:C:H5'    | 2.10                     | 0.52              |
| 27:DA:1779:U:O4   | 27:DA:1785:A:C6    | 2.62                     | 0.52              |
| 27:DA:1963:U:O2   | 27:DA:1963:U:H2'   | 2.09                     | 0.52              |
| 27:DA:1991:U:H2'  | 27:DA:1992:G:C5'   | 2.38                     | 0.52              |
| 27:DA:2001:A:H2'  | 27:DA:2002:G:O4'   | 2.10                     | 0.52              |
| 27:DA:1493:C:C5   | 27:DA:2206:G:O2'   | 2.63                     | 0.52              |
| 27:DA:247:G:O6    | 57:D8:12:LYS:HE3   | 2.10                     | 0.52              |
| 27:DA:2719:G:H5'  | 27:DA:2847:U:OP1   | 2.10                     | 0.52              |
| 27:DA:319:C:C2    | 27:DA:333:G:N2     | 2.78                     | 0.52              |
| 34:DH:140:LYS:O   | 34:DH:144:VAL:HG23 | 2.10                     | 0.52              |
| 34:DH:32:GLU:O    | 34:DH:33:LEU:HD23  | 2.09                     | 0.52              |
| 34:DH:85:LYS:CG   | 34:DH:133:VAL:HB   | 2.40                     | 0.52              |
| 38:DP:122:PRO:HA  | 38:DP:141:ALA:O    | 2.09                     | 0.52              |
| 38:DP:9:ASN:ND2   | 38:DP:10:PRO:CD    | 2.61                     | 0.52              |
| 41:DS:56:LEU:O    | 41:DS:57:LYS:HB2   | 2.09                     | 0.52              |
| 42:DT:57:PHE:O    | 42:DT:58:ASN:C     | 2.47                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:19:C:OP1     | 43:DU:22:LYS:CD   | 2.55                     | 0.52              |
| 46:DX:64:LYS:NZ    | 46:DX:73:ARG:CZ   | 2.72                     | 0.52              |
| 48:DZ:107:PRO:C    | 48:DZ:109:GLY:N   | 2.62                     | 0.52              |
| 48:DZ:108:ALA:O    | 48:DZ:144:GLU:HG2 | 2.10                     | 0.52              |
| 48:DZ:23:LEU:HD21  | 48:DZ:85:VAL:HG13 | 1.91                     | 0.52              |
| 1:AA:108:G:C6      | 20:AT:15:ARG:HD2  | 2.45                     | 0.52              |
| 1:AA:1199:U:H4'    | 10:AJ:54:PHE:CE2  | 2.45                     | 0.52              |
| 1:AA:1243:C:O2'    | 1:AA:1244:C:H5'   | 2.09                     | 0.52              |
| 1:AA:186:C:H2'     | 1:AA:187:C:C6     | 2.45                     | 0.52              |
| 1:AA:265:G:H21     | 1:AA:267:C:H5'    | 1.75                     | 0.52              |
| 1:AA:686:U:HO2'    | 1:AA:687:A:H8     | 1.51                     | 0.52              |
| 1:AA:848:C:H2'     | 1:AA:849:C:C6     | 2.44                     | 0.52              |
| 1:AA:935:A:H61     | 7:AG:3:ARG:HB2    | 1.74                     | 0.52              |
| 4:AD:68:TYR:HA     | 4:AD:114:ARG:CD   | 2.40                     | 0.52              |
| 5:AE:53:LEU:N      | 5:AE:53:LEU:HD12  | 2.25                     | 0.52              |
| 6:AF:61:LEU:O      | 6:AF:62:TRP:CB    | 2.57                     | 0.52              |
| 7:AG:15:ASP:HB3    | 7:AG:20:ASP:H     | 1.75                     | 0.52              |
| 8:AH:39:LEU:HB3    | 8:AH:45:ILE:HG12  | 1.92                     | 0.52              |
| 8:AH:60:ARG:CG     | 8:AH:60:ARG:NH1   | 2.68                     | 0.52              |
| 12:AL:23:ALA:C     | 12:AL:24:LEU:HD22 | 2.30                     | 0.52              |
| 15:AO:39:LEU:C     | 15:AO:41:GLU:H    | 2.13                     | 0.52              |
| 16:AP:50:LYS:HD3   | 16:AP:51:VAL:N    | 2.24                     | 0.52              |
| 19:AS:44:MET:SD    | 19:AS:44:MET:N    | 2.83                     | 0.52              |
| 20:AT:98:PRO:C     | 20:AT:100:ILE:N   | 2.62                     | 0.52              |
| 50:B1:20:ARG:HA    | 50:B1:34:THR:HA   | 1.92                     | 0.52              |
| 50:B1:64:ALA:HA    | 50:B1:67:ILE:CG1  | 2.39                     | 0.52              |
| 27:BA:1311:G:C4    | 56:B7:47:ARG:NH2  | 2.78                     | 0.52              |
| 27:BA:1209:G:O2'   | 27:BA:1237:A:N1   | 2.31                     | 0.52              |
| 27:BA:1310:G:N2    | 27:BA:1313:U:O4   | 2.43                     | 0.52              |
| 27:BA:1682:G:C6    | 27:BA:1683:C:N3   | 2.78                     | 0.52              |
| 27:BA:2273:A:H2'   | 27:BA:2274:A:C8   | 2.45                     | 0.52              |
| 27:BA:2302:G:H2'   | 27:BA:2303:G:H5'  | 1.92                     | 0.52              |
| 27:BA:2580:U:H4'   | 31:BE:130:GLY:HA2 | 1.92                     | 0.52              |
| 27:BA:26:G:C2'     | 27:BA:514:A:H61   | 2.22                     | 0.52              |
| 27:BA:397:G:O2'    | 27:BA:398:G:H5'   | 2.09                     | 0.52              |
| 27:BA:937:U:H2'    | 27:BA:938:G:C8    | 2.44                     | 0.52              |
| 28:BB:61:G:C2      | 28:BB:62:C:C2     | 2.98                     | 0.52              |
| 31:BE:119:ARG:HD2  | 31:BE:120:TRP:CD1 | 2.45                     | 0.52              |
| 32:BF:176:LEU:HD12 | 32:BF:177:ALA:N   | 2.23                     | 0.52              |
| 32:BF:188:ARG:HB2  | 38:BP:7:ARG:HH22  | 1.74                     | 0.52              |
| 35:BI:76:THR:O     | 35:BI:140:LEU:HA  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BI:91:SER:HB2  | 35:BI:119:PRO:HB2  | 1.90                     | 0.52              |
| 37:BO:17:ARG:HE   | 37:BO:47:ILE:CD1   | 2.23                     | 0.52              |
| 37:BO:25:LEU:O    | 37:BO:26:LYS:HG3   | 2.09                     | 0.52              |
| 27:BA:251:A:H5''  | 38:BP:51:PHE:HZ    | 1.75                     | 0.52              |
| 41:BS:54:LEU:C    | 41:BS:56:LEU:H     | 2.13                     | 0.52              |
| 43:BU:61:TRP:O    | 43:BU:62:ILE:C     | 2.48                     | 0.52              |
| 44:BV:35:LEU:C    | 44:BV:37:VAL:H     | 2.13                     | 0.52              |
| 47:BY:84:ARG:O    | 47:BY:94:LYS:HA    | 2.09                     | 0.52              |
| 1:CA:1086:U:H3'   | 1:CA:1087:G:H8     | 1.75                     | 0.52              |
| 1:CA:1404:C:O4'   | 1:CA:1499:A:C2     | 2.63                     | 0.52              |
| 1:CA:376:G:OP1    | 16:CP:5:ARG:HB2    | 2.08                     | 0.52              |
| 1:CA:386:C:C2'    | 1:CA:387:U:C5'     | 2.81                     | 0.52              |
| 1:CA:59:A:H5''    | 1:CA:60:A:C5'      | 2.40                     | 0.52              |
| 3:CC:182:ILE:HG23 | 3:CC:202:ILE:O     | 2.09                     | 0.52              |
| 10:CJ:90:LEU:N    | 10:CJ:91:PRO:CD    | 2.73                     | 0.52              |
| 12:CL:5:ASN:HD22  | 17:CQ:34:LYS:HZ3   | 1.58                     | 0.52              |
| 1:CA:1310:G:C5'   | 13:CM:77:ASN:ND2   | 2.72                     | 0.52              |
| 13:CM:91:ARG:CB   | 13:CM:98:VAL:HG13  | 2.40                     | 0.52              |
| 24:CX:29:G:C2'    | 24:CX:30:G:H5'     | 2.40                     | 0.52              |
| 24:CX:15:G:H2'    | 24:CX:59:A:N1      | 2.24                     | 0.52              |
| 51:D2:33:MET:O    | 51:D2:34:GLU:C     | 2.48                     | 0.52              |
| 51:D2:5:GLU:O     | 51:D2:8:LYS:HB2    | 2.10                     | 0.52              |
| 53:D4:41:ILE:HD13 | 53:D4:47:VAL:HG13  | 1.91                     | 0.52              |
| 53:D4:42:CYS:SG   | 53:D4:46:ASN:O     | 2.68                     | 0.52              |
| 33:DG:105:LYS:HE3 | 53:D4:51:TYR:O     | 2.10                     | 0.52              |
| 27:DA:1368:G:O2'  | 27:DA:1369:G:H5'   | 2.10                     | 0.52              |
| 27:DA:1651:G:C2   | 27:DA:2007:C:N3    | 2.78                     | 0.52              |
| 27:DA:2057:A:H2'  | 27:DA:2058:A:O4'   | 2.09                     | 0.52              |
| 27:DA:2350:C:H41  | 27:DA:2382:G:H22   | 1.58                     | 0.52              |
| 27:DA:262:A:H2'   | 27:DA:263:C:C6     | 2.45                     | 0.52              |
| 27:DA:2756:U:C1'  | 27:DA:2757:A:H5''  | 2.35                     | 0.52              |
| 28:DB:79:C:H2'    | 28:DB:80:U:O4'     | 2.10                     | 0.52              |
| 29:DC:214:VAL:C   | 29:DC:216:THR:N    | 2.61                     | 0.52              |
| 30:DD:15:PHE:O    | 30:DD:17:THR:HG23  | 2.10                     | 0.52              |
| 30:DD:261:LYS:NZ  | 30:DD:263:ARG:HH12 | 2.04                     | 0.52              |
| 30:DD:55:GLY:HA3  | 30:DD:218:ARG:HD3  | 1.91                     | 0.52              |
| 30:DD:94:LEU:HD22 | 30:DD:95:LEU:N     | 2.25                     | 0.52              |
| 31:DE:113:PHE:HD2 | 31:DE:113:PHE:C    | 2.13                     | 0.52              |
| 31:DE:35:GLN:HA   | 31:DE:67:PHE:CZ    | 2.45                     | 0.52              |
| 34:DH:27:LYS:HG2  | 34:DH:32:GLU:CG    | 2.39                     | 0.52              |
| 36:DN:26:LEU:HG   | 36:DN:30:ILE:HD11  | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DX:30:VAL:HG23  | 46:DX:77:LYS:HB3   | 1.90                     | 0.52              |
| 47:DY:39:VAL:CG1   | 47:DY:40:GLU:H     | 2.07                     | 0.52              |
| 48:DZ:126:LYS:HD3  | 48:DZ:161:GLU:OE1  | 2.10                     | 0.52              |
| 1:AA:1028:C:C2'    | 1:AA:1029:C:H5'    | 2.40                     | 0.52              |
| 1:AA:1088:G:O2'    | 1:AA:1089:G:H5'    | 2.10                     | 0.52              |
| 1:AA:1340:A:O2'    | 1:AA:1341:U:H5'    | 2.10                     | 0.52              |
| 1:AA:189(I):G:H2'  | 1:AA:189(J):G:H8   | 1.74                     | 0.52              |
| 1:AA:324:G:H21     | 1:AA:327:A:H8      | 1.56                     | 0.52              |
| 1:AA:33:A:H2'      | 1:AA:34:C:C6       | 2.45                     | 0.52              |
| 1:AA:375:U:H4'     | 16:AP:17:TYR:CE2   | 2.45                     | 0.52              |
| 1:AA:41:G:O2'      | 1:AA:42:G:H5'      | 2.10                     | 0.52              |
| 1:AA:503:C:H2'     | 1:AA:504:C:C6      | 2.42                     | 0.52              |
| 1:AA:532:A:H3'     | 1:AA:533:A:H5''    | 1.89                     | 0.52              |
| 2:AB:69:LEU:HD12   | 2:AB:69:LEU:C      | 2.30                     | 0.52              |
| 3:AC:47:LEU:HD21   | 3:AC:68:VAL:HG11   | 1.91                     | 0.52              |
| 5:AE:33:VAL:HG11   | 5:AE:109:ILE:HG12  | 1.92                     | 0.52              |
| 7:AG:27:ILE:O      | 7:AG:30:ILE:HG12   | 2.10                     | 0.52              |
| 16:AP:58:TYR:CD1   | 16:AP:58:TYR:C     | 2.83                     | 0.52              |
| 19:AS:6:LYS:HG2    | 19:AS:7:LYS:HE3    | 1.92                     | 0.52              |
| 20:AT:80:ARG:O     | 20:AT:84:LEU:N     | 2.41                     | 0.52              |
| 51:B2:32:LEU:O     | 51:B2:35:LEU:HB2   | 2.10                     | 0.52              |
| 57:B8:14:VAL:HG21  | 57:B8:22:VAL:CG1   | 2.40                     | 0.52              |
| 57:B8:32:LEU:HB3   | 57:B8:36:LYS:CD    | 2.40                     | 0.52              |
| 58:B9:18:ARG:NH1   | 58:B9:21:GLY:HA2   | 2.24                     | 0.52              |
| 27:BA:1614:A:H62   | 45:BW:93:ALA:HB2   | 1.75                     | 0.52              |
| 27:BA:1828:G:H4'   | 27:BA:1829:A:OP1   | 2.10                     | 0.52              |
| 27:BA:2420:C:P     | 57:B8:33:ASN:O     | 2.68                     | 0.52              |
| 27:BA:323:G:H5'    | 32:BF:169:ASN:HD21 | 1.75                     | 0.52              |
| 27:BA:335:C:OP1    | 27:BA:335:C:H6     | 1.93                     | 0.52              |
| 27:BA:382:G:H1     | 27:BA:392:C:H42    | 1.58                     | 0.52              |
| 27:BA:671:C:C6     | 27:BA:671:C:H5'    | 2.44                     | 0.52              |
| 27:BA:76:C:C2      | 27:BA:111:A:C2     | 2.98                     | 0.52              |
| 27:BA:816:C:O2'    | 27:BA:817:C:H5'    | 2.09                     | 0.52              |
| 29:BC:36:LYS:O     | 29:BC:37:PHE:C     | 2.48                     | 0.52              |
| 30:BD:94:LEU:HB2   | 30:BD:104:TYR:HE2  | 1.75                     | 0.52              |
| 30:BD:44:ASN:ND2   | 30:BD:47:GLY:O     | 2.41                     | 0.52              |
| 27:BA:2784:C:C1'   | 31:BE:42:ASP:OD1   | 2.48                     | 0.52              |
| 32:BF:126:VAL:HG21 | 32:BF:129:PHE:CE1  | 2.45                     | 0.52              |
| 32:BF:53:THR:HG22  | 32:BF:55:GLY:H     | 1.75                     | 0.52              |
| 33:BG:123:ASN:O    | 33:BG:125:PHE:N    | 2.42                     | 0.52              |
| 33:BG:60:LEU:O     | 33:BG:60:LEU:HD13  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BH:126:PRO:O   | 34:BH:127:GLU:CB  | 2.54                     | 0.52              |
| 34:BH:40:GLU:O    | 34:BH:41:MET:HB2  | 2.10                     | 0.52              |
| 34:BH:73:ALA:O    | 34:BH:76:VAL:HG23 | 2.09                     | 0.52              |
| 35:BI:69:LYS:O    | 35:BI:73:GLU:HB3  | 2.10                     | 0.52              |
| 36:BN:18:ALA:HB1  | 36:BN:21:LYS:HB3  | 1.92                     | 0.52              |
| 37:BO:14:THR:HG22 | 37:BO:16:ALA:N    | 2.25                     | 0.52              |
| 41:BS:38:GLN:HA   | 41:BS:50:SER:HA   | 1.92                     | 0.52              |
| 42:BT:82:LEU:O    | 42:BT:83:ILE:C    | 2.48                     | 0.52              |
| 44:BV:39:LEU:HB3  | 44:BV:47:VAL:HG11 | 1.91                     | 0.52              |
| 45:BW:33:ARG:HG3  | 45:BW:33:ARG:HH11 | 1.74                     | 0.52              |
| 47:BY:95:LYS:HA   | 47:BY:100:ALA:HA  | 1.92                     | 0.52              |
| 1:CA:66:G:N7      | 1:CA:104:G:N2     | 2.58                     | 0.52              |
| 1:CA:1474:G:H4'   | 27:DA:1701:A:N3   | 2.25                     | 0.52              |
| 1:CA:1504:G:H1'   | 1:CA:1505:G:OP2   | 2.09                     | 0.52              |
| 1:CA:645:C:H2'    | 1:CA:646:U:H6     | 1.74                     | 0.52              |
| 1:CA:742:G:OP1    | 15:CO:35:ARG:NH2  | 2.42                     | 0.52              |
| 1:CA:838:G:N2     | 1:CA:840:C:H5'    | 2.24                     | 0.52              |
| 2:CB:165:VAL:HG23 | 2:CB:166:ASP:N    | 2.25                     | 0.52              |
| 2:CB:224:GLN:HG2  | 2:CB:229:VAL:HG22 | 1.92                     | 0.52              |
| 2:CB:95:GLN:O     | 2:CB:96:ARG:C     | 2.48                     | 0.52              |
| 4:CD:10:ARG:HG3   | 4:CD:40:PRO:HB3   | 1.92                     | 0.52              |
| 9:CI:4:TYR:HA     | 9:CI:88:TYR:CE1   | 2.45                     | 0.52              |
| 1:CA:963:G:N2     | 10:CJ:55:LYS:HZ2  | 2.08                     | 0.52              |
| 10:CJ:48:THR:CG2  | 10:CJ:62:HIS:HB3  | 2.35                     | 0.52              |
| 10:CJ:82:ILE:HD13 | 10:CJ:85:LEU:HD12 | 1.90                     | 0.52              |
| 11:CK:110:ASP:O   | 18:CR:84:LYS:HG3  | 2.10                     | 0.52              |
| 11:CK:12:ARG:O    | 11:CK:13:GLN:HG3  | 2.10                     | 0.52              |
| 14:CN:7:ILE:HG13  | 14:CN:8:GLU:N     | 2.23                     | 0.52              |
| 1:CA:189(F):U:H5  | 17:CQ:3:LYS:HZ3   | 1.58                     | 0.52              |
| 19:CS:17:GLU:O    | 19:CS:21:GLU:HG3  | 2.10                     | 0.52              |
| 19:CS:18:LYS:O    | 19:CS:22:LEU:HD23 | 2.10                     | 0.52              |
| 19:CS:40:ILE:HB   | 19:CS:67:VAL:O    | 2.09                     | 0.52              |
| 53:D4:48:ILE:HD12 | 53:D4:48:ILE:N    | 2.24                     | 0.52              |
| 57:D8:50:LEU:HD12 | 57:D8:51:ALA:H    | 1.72                     | 0.52              |
| 27:DA:1374:G:H2'  | 27:DA:1375:C:H6   | 1.74                     | 0.52              |
| 27:DA:1378:A:C4'  | 27:DA:1379:A:OP1  | 2.55                     | 0.52              |
| 27:DA:1505:C:C5   | 27:DA:1506:C:H1'  | 2.45                     | 0.52              |
| 27:DA:1771:C:C2   | 27:DA:1772:G:C8   | 2.97                     | 0.52              |
| 27:DA:1792:G:H2'  | 27:DA:1793:C:C6   | 2.45                     | 0.52              |
| 27:DA:1972:A:H2'  | 27:DA:1973:G:H8   | 1.75                     | 0.52              |
| 27:DA:2496:C:OP2  | 39:DQ:82:ARG:NE   | 2.42                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:2848:G:H3'  | 42:DT:95:ARG:O     | 2.10                     | 0.52              |
| 27:DA:2882:A:OP1  | 40:DR:96:ARG:HD3   | 2.10                     | 0.52              |
| 27:DA:333:G:C4    | 27:DA:334:C:C5     | 2.98                     | 0.52              |
| 27:DA:832:G:O2'   | 38:DP:52:GLU:HB3   | 2.10                     | 0.52              |
| 31:DE:167:VAL:CG2 | 31:DE:170:LEU:HD11 | 2.40                     | 0.52              |
| 27:DA:2636:U:HO2' | 31:DE:44:TYR:HH    | 1.52                     | 0.52              |
| 32:DF:39:TRP:O    | 32:DF:43:LYS:HG2   | 2.10                     | 0.52              |
| 28:DB:55:U:O3'    | 33:DG:27:ASN:OD1   | 2.24                     | 0.52              |
| 34:DH:138:LYS:O   | 34:DH:141:VAL:HB   | 2.10                     | 0.52              |
| 35:DI:133:HIS:ND1 | 35:DI:134:PRO:HD3  | 2.25                     | 0.52              |
| 27:DA:626:U:H3    | 38:DP:105:LEU:HB3  | 1.75                     | 0.52              |
| 39:DQ:27:VAL:HG12 | 39:DQ:28:ALA:N     | 2.24                     | 0.52              |
| 48:DZ:74:ASN:O    | 48:DZ:83:GLU:HB2   | 2.10                     | 0.52              |
| 1:AA:1066:C:O2'   | 1:AA:1067:A:H5'    | 2.11                     | 0.51              |
| 1:AA:1363:C:H5'   | 1:AA:1363(A):A:O5' | 2.10                     | 0.51              |
| 1:AA:495:A:C4'    | 1:AA:496:A:H5''    | 2.35                     | 0.51              |
| 1:AA:909:A:H2'    | 1:AA:910:C:C5'     | 2.40                     | 0.51              |
| 9:AI:21:PRO:HA    | 9:AI:59:PHE:HA     | 1.92                     | 0.51              |
| 12:AL:56:ARG:HA   | 12:AL:62:GLU:HG3   | 1.93                     | 0.51              |
| 13:AM:66:LEU:O    | 13:AM:69:GLU:O     | 2.28                     | 0.51              |
| 26:AZ:4:SER:H     | 27:BA:1913:A:HO2'  | 1.58                     | 0.51              |
| 54:B5:47:PRO:O    | 54:B5:48:GLU:HG3   | 2.10                     | 0.51              |
| 27:BA:1279:G:N2   | 27:BA:1292:U:C2    | 2.78                     | 0.51              |
| 27:BA:1615:C:C6   | 27:BA:1617:C:C5    | 2.99                     | 0.51              |
| 27:BA:2576:G:H5'  | 27:BA:2579:C:H41   | 1.75                     | 0.51              |
| 27:BA:431:U:O5'   | 27:BA:431:U:H6     | 1.92                     | 0.51              |
| 27:BA:534:U:H2'   | 27:BA:535:C:H6     | 1.75                     | 0.51              |
| 30:BD:35:LYS:NZ   | 30:BD:103:ARG:N    | 2.58                     | 0.51              |
| 30:BD:44:ASN:N    | 30:BD:44:ASN:OD1   | 2.43                     | 0.51              |
| 31:BE:4:ILE:HG12  | 31:BE:28:ALA:HB1   | 1.93                     | 0.51              |
| 31:BE:57:LYS:HB3  | 31:BE:57:LYS:NZ    | 2.23                     | 0.51              |
| 32:BF:123:LEU:CD1 | 32:BF:124:LEU:N    | 2.71                     | 0.51              |
| 27:BA:1140:C:P    | 36:BN:66:LYS:HZ1   | 2.32                     | 0.51              |
| 38:BP:63:PRO:O    | 38:BP:64:LYS:C     | 2.48                     | 0.51              |
| 39:BQ:5:ARG:O     | 39:BQ:6:ARG:HB2    | 2.08                     | 0.51              |
| 42:BT:6:LEU:O     | 42:BT:10:VAL:HG23  | 2.10                     | 0.51              |
| 44:BV:57:VAL:CG1  | 44:BV:57:VAL:O     | 2.59                     | 0.51              |
| 46:BX:41:ASN:O    | 46:BX:45:THR:HG23  | 2.11                     | 0.51              |
| 47:BY:47:LYS:N    | 47:BY:47:LYS:HD2   | 2.25                     | 0.51              |
| 48:BZ:73:VAL:HG22 | 48:BZ:85:VAL:HG12  | 1.92                     | 0.51              |
| 1:CA:1226:C:C5    | 13:CM:104:ARG:CA   | 2.90                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:929:G:N2      | 1:CA:1389:C:C2     | 2.78                     | 0.51              |
| 1:CA:428:G:O2'     | 1:CA:429:U:P       | 2.68                     | 0.51              |
| 1:CA:552:U:H4'     | 12:CL:83:ARG:CG    | 2.40                     | 0.51              |
| 1:CA:57:G:H2'      | 1:CA:58:C:H6       | 1.69                     | 0.51              |
| 2:CB:109:SER:HA    | 2:CB:112:VAL:HG23  | 1.92                     | 0.51              |
| 3:CC:188:LEU:O     | 3:CC:189:ALA:CB    | 2.57                     | 0.51              |
| 4:CD:6:GLY:O       | 4:CD:7:PRO:C       | 2.48                     | 0.51              |
| 5:CE:10:MET:HB2    | 5:CE:32:VAL:CG2    | 2.40                     | 0.51              |
| 7:CG:113:GLU:HB2   | 7:CG:119:ARG:CG    | 2.21                     | 0.51              |
| 9:CI:93:ARG:C      | 9:CI:95:LYS:H      | 2.13                     | 0.51              |
| 12:CL:107:VAL:HG11 | 12:CL:110:ARG:HB2  | 1.91                     | 0.51              |
| 12:CL:82:ILE:HG21  | 12:CL:95:TYR:HD2   | 1.75                     | 0.51              |
| 13:CM:105:THR:O    | 13:CM:106:ASN:HB2  | 2.10                     | 0.51              |
| 1:CA:1310:G:H5''   | 13:CM:77:ASN:HD21  | 1.75                     | 0.51              |
| 16:CP:81:ARG:HG2   | 16:CP:83:GLU:OE2   | 2.10                     | 0.51              |
| 20:CT:104:LEU:HD23 | 20:CT:105:SER:H    | 1.75                     | 0.51              |
| 23:CW:23:G:H2'     | 23:CW:24:C:C6      | 2.45                     | 0.51              |
| 24:CX:28:C:N4      | 24:CX:42:G:H1      | 2.08                     | 0.51              |
| 50:D1:82:LEU:C     | 50:D1:83:GLU:CD    | 2.68                     | 0.51              |
| 54:D5:25:LEU:HD22  | 54:D5:26:THR:H     | 1.70                     | 0.51              |
| 27:DA:1267:U:HO2'  | 27:DA:1268:A:H8    | 0.69                     | 0.51              |
| 27:DA:2328:A:H2'   | 27:DA:2329:G:O4'   | 2.10                     | 0.51              |
| 27:DA:2061:G:H5''  | 27:DA:2503:A:N1    | 2.26                     | 0.51              |
| 27:DA:2582:G:O2'   | 27:DA:2583:G:H5'   | 2.08                     | 0.51              |
| 27:DA:2887:U:O2'   | 27:DA:2888:C:H5'   | 2.09                     | 0.51              |
| 27:DA:290:G:O2'    | 27:DA:291:C:H5'    | 2.10                     | 0.51              |
| 27:DA:614(A):U:H4' | 27:DA:614(B):G:O5' | 2.10                     | 0.51              |
| 27:DA:747:U:H6     | 27:DA:747:U:O5'    | 1.92                     | 0.51              |
| 27:DA:1993:U:C5'   | 31:DE:128:SER:HB3  | 2.40                     | 0.51              |
| 33:DG:6:ALA:HB3    | 33:DG:104:GLU:OE1  | 2.10                     | 0.51              |
| 38:DP:144:GLU:O    | 38:DP:146:VAL:N    | 2.44                     | 0.51              |
| 38:DP:96:THR:O     | 38:DP:99:LEU:HB3   | 2.10                     | 0.51              |
| 39:DQ:133:ARG:HH11 | 39:DQ:133:ARG:HG3  | 1.75                     | 0.51              |
| 27:DA:870:A:P      | 39:DQ:6:ARG:HH21   | 2.32                     | 0.51              |
| 40:DR:96:ARG:O     | 40:DR:114:VAL:HA   | 2.10                     | 0.51              |
| 41:DS:26:LEU:HD12  | 41:DS:85:VAL:HG21  | 1.92                     | 0.51              |
| 42:DT:28:VAL:CG1   | 42:DT:46:GLU:HG3   | 2.39                     | 0.51              |
| 45:DW:69:LEU:O     | 45:DW:110:LYS:NZ   | 2.42                     | 0.51              |
| 48:DZ:143:LEU:O    | 48:DZ:173:VAL:HG21 | 2.10                     | 0.51              |
| 48:DZ:76:ASP:HB2   | 48:DZ:83:GLU:HG2   | 1.92                     | 0.51              |
| 1:AA:1007:C:H2'    | 1:AA:1008:C:C6     | 2.45                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1154:G:O2'    | 1:AA:1155:G:O4'    | 2.27                     | 0.51              |
| 1:AA:1053:G:HO2'   | 1:AA:1199:U:H5     | 1.58                     | 0.51              |
| 1:AA:161:A:H2'     | 1:AA:162:A:O4'     | 2.10                     | 0.51              |
| 1:AA:267:C:P       | 17:AQ:67:LYS:HB2   | 2.50                     | 0.51              |
| 1:AA:441:A:H3'     | 1:AA:442:C:C6      | 2.38                     | 0.51              |
| 3:AC:142:MET:HE1   | 3:AC:171:GLY:HA3   | 1.91                     | 0.51              |
| 3:AC:201:TYR:O     | 3:AC:202:ILE:HD13  | 2.10                     | 0.51              |
| 5:AE:79:GLU:HA     | 5:AE:91:LEU:O      | 2.10                     | 0.51              |
| 9:AI:106:ALA:O     | 9:AI:107:ARG:C     | 2.48                     | 0.51              |
| 1:AA:1291:G:H4'    | 9:AI:38:GLN:O      | 2.10                     | 0.51              |
| 10:AJ:50:ILE:CD1   | 10:AJ:60:ARG:HD3   | 2.40                     | 0.51              |
| 13:AM:28:ALA:O     | 13:AM:32:GLU:N     | 2.43                     | 0.51              |
| 1:AA:1319:A:OP1    | 19:AS:10:PHE:CZ    | 2.64                     | 0.51              |
| 20:AT:63:ILE:HG22  | 20:AT:77:ALA:HB1   | 1.92                     | 0.51              |
| 21:AU:5:ASP:O      | 21:AU:11:GLY:HA3   | 2.10                     | 0.51              |
| 51:B2:14:ARG:HG3   | 51:B2:14:ARG:NH1   | 2.25                     | 0.51              |
| 27:BA:1202:C:C2    | 27:BA:1244:G:N2    | 2.78                     | 0.51              |
| 27:BA:1328:G:H2'   | 27:BA:1330:C:C4    | 2.45                     | 0.51              |
| 27:BA:1385:G:O2'   | 27:BA:1386:C:H6    | 1.92                     | 0.51              |
| 27:BA:1442:G:C2    | 27:BA:1550:C:O2    | 2.63                     | 0.51              |
| 27:BA:2192:G:H2'   | 27:BA:2193:G:H5'   | 1.91                     | 0.51              |
| 27:BA:2243:U:O2'   | 27:BA:2244:U:H5'   | 2.11                     | 0.51              |
| 27:BA:2569:G:O2'   | 27:BA:2570:G:H5'   | 2.10                     | 0.51              |
| 27:BA:271(B):C:C2' | 27:BA:271(C):C:H5' | 2.40                     | 0.51              |
| 27:BA:284:U:O2'    | 27:BA:285:C:H5'    | 2.10                     | 0.51              |
| 27:BA:665:C:O2'    | 27:BA:666:G:H5'    | 2.09                     | 0.51              |
| 27:BA:684:G:C2     | 27:BA:774:A:C2     | 2.97                     | 0.51              |
| 27:BA:887:A:O2'    | 27:BA:888:C:H5''   | 2.10                     | 0.51              |
| 30:BD:24:ILE:O     | 30:BD:26:LYS:CE    | 2.58                     | 0.51              |
| 31:BE:7:VAL:HG23   | 31:BE:8:LYS:O      | 2.09                     | 0.51              |
| 32:BF:168:ARG:HG2  | 32:BF:175:THR:HG21 | 1.90                     | 0.51              |
| 35:BI:132:PRO:HD2  | 35:BI:133:HIS:HD2  | 1.72                     | 0.51              |
| 35:BI:136:VAL:O    | 35:BI:138:ILE:HG12 | 2.10                     | 0.51              |
| 36:BN:62:VAL:HG22  | 36:BN:63:THR:N     | 2.25                     | 0.51              |
| 37:BO:8:LEU:HD12   | 37:BO:82:ASN:HB3   | 1.90                     | 0.51              |
| 39:BQ:81:VAL:HG23  | 39:BQ:82:ARG:N     | 2.24                     | 0.51              |
| 41:BS:66:ALA:O     | 41:BS:69:VAL:HG12  | 2.11                     | 0.51              |
| 42:BT:108:ARG:HA   | 42:BT:111:ARG:HD3  | 1.92                     | 0.51              |
| 44:BV:17:GLY:HA2   | 44:BV:96:ILE:HB    | 1.93                     | 0.51              |
| 27:BA:1339:G:OP1   | 46:BX:14:SER:CB    | 2.57                     | 0.51              |
| 1:CA:1307:U:C2'    | 1:CA:1308:U:H6     | 2.23                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1346:A:N6    | 1:CA:1374:A:H3'   | 2.17                     | 0.51              |
| 1:CA:197:A:H1'    | 1:CA:198:G:O4'    | 2.10                     | 0.51              |
| 1:CA:477:A:C2'    | 1:CA:479:C:H5'    | 2.41                     | 0.51              |
| 1:CA:532:A:O2'    | 1:CA:533:A:C5'    | 2.59                     | 0.51              |
| 3:CC:119:ARG:HH11 | 3:CC:119:ARG:HG3  | 1.75                     | 0.51              |
| 3:CC:87:LEU:C     | 3:CC:89:GLU:N     | 2.62                     | 0.51              |
| 4:CD:11:LEU:N     | 4:CD:11:LEU:HD23  | 2.24                     | 0.51              |
| 4:CD:198:VAL:CG1  | 4:CD:199:ASN:H    | 2.21                     | 0.51              |
| 4:CD:49:ARG:HD3   | 4:CD:50:ARG:H     | 1.74                     | 0.51              |
| 4:CD:94:LEU:HA    | 4:CD:97:LEU:HD12  | 1.92                     | 0.51              |
| 5:CE:106:PRO:O    | 5:CE:110:LEU:HG   | 2.10                     | 0.51              |
| 5:CE:78:HIS:C     | 5:CE:93:PRO:HD3   | 2.29                     | 0.51              |
| 7:CG:123:GLU:O    | 7:CG:127:ALA:HB2  | 2.11                     | 0.51              |
| 1:CA:1280:A:C5'   | 10:CJ:40:LEU:HD12 | 2.38                     | 0.51              |
| 12:CL:15:VAL:CG2  | 12:CL:16:ARG:H    | 2.05                     | 0.51              |
| 13:CM:36:LYS:NZ   | 13:CM:59:TYR:HE1  | 2.05                     | 0.51              |
| 52:D3:39:ASP:CG   | 52:D3:44:ARG:HE   | 2.13                     | 0.51              |
| 27:DA:1314:C:H2'  | 27:DA:1315:C:H6   | 1.76                     | 0.51              |
| 27:DA:1625:C:H2'  | 27:DA:1626:G:C5'  | 2.39                     | 0.51              |
| 27:DA:2033:A:C5   | 27:DA:2036:C:C4   | 2.97                     | 0.51              |
| 27:DA:2145:C:H4'  | 27:DA:2146:C:OP2  | 2.10                     | 0.51              |
| 27:DA:2553:G:C6   | 27:DA:2554:U:O2   | 2.64                     | 0.51              |
| 27:DA:2632:A:H2   | 31:DE:61:ARG:HD3  | 1.74                     | 0.51              |
| 27:DA:360:G:O2'   | 27:DA:361:G:H5'   | 2.09                     | 0.51              |
| 27:DA:557:U:O2'   | 27:DA:558:G:H5'   | 2.09                     | 0.51              |
| 27:DA:567:A:H2'   | 27:DA:568:U:O5'   | 2.10                     | 0.51              |
| 27:DA:593:G:O2'   | 27:DA:594:U:H5'   | 2.10                     | 0.51              |
| 27:DA:668:G:C4    | 27:DA:670:A:C5    | 2.99                     | 0.51              |
| 27:DA:84:A:OP2    | 47:DY:9:LYS:NZ    | 2.44                     | 0.51              |
| 27:DA:857:C:H5'   | 49:D0:77:ARG:NH1  | 2.21                     | 0.51              |
| 27:DA:919:G:H4'   | 28:DB:81:G:H4'    | 1.92                     | 0.51              |
| 29:DC:68:LEU:HD11 | 29:DC:179:SER:CA  | 2.39                     | 0.51              |
| 30:DD:233:HIS:CE1 | 30:DD:246:PRO:HA  | 2.44                     | 0.51              |
| 32:DF:37:VAL:HG12 | 32:DF:41:LEU:HD12 | 1.91                     | 0.51              |
| 33:DG:150:ASP:OD1 | 33:DG:153:ARG:NH2 | 2.42                     | 0.51              |
| 37:DO:107:ARG:HG3 | 37:DO:112:MET:SD  | 2.50                     | 0.51              |
| 40:DR:100:LEU:CD2 | 40:DR:113:LEU:HB2 | 2.39                     | 0.51              |
| 46:DX:65:ARG:HB2  | 46:DX:70:LEU:HG   | 1.91                     | 0.51              |
| 47:DY:43:ASN:O    | 47:DY:44:ILE:O    | 2.28                     | 0.51              |
| 1:AA:1033:G:C2'   | 1:AA:1034:G:H5'   | 2.40                     | 0.51              |
| 1:AA:228:A:H2'    | 1:AA:229:U:O4'    | 2.11                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:646:U:O2'     | 1:AA:647:C:H5'    | 2.11                     | 0.51              |
| 1:AA:817:C:H4'     | 1:AA:818:G:OP1    | 2.06                     | 0.51              |
| 1:AA:1314:C:H5     | 19:AS:6:LYS:NZ    | 2.08                     | 0.51              |
| 24:AX:74:C:C2'     | 24:AX:75:C:H5'    | 2.39                     | 0.51              |
| 51:B2:33:MET:O     | 51:B2:35:LEU:N    | 2.43                     | 0.51              |
| 27:BA:851:U:O2'    | 52:B3:45:GLY:HA3  | 2.10                     | 0.51              |
| 54:B5:34:PRO:C     | 54:B5:36:CYS:H    | 2.13                     | 0.51              |
| 27:BA:1449:A:H5'   | 27:BA:1450:G:OP2  | 2.09                     | 0.51              |
| 27:BA:1829:A:H2'   | 27:BA:1830:C:H5'  | 1.92                     | 0.51              |
| 27:BA:2008:C:O2'   | 27:BA:2009:G:H5'  | 2.10                     | 0.51              |
| 27:BA:2099:U:H3    | 27:BA:2190:G:H1   | 1.58                     | 0.51              |
| 27:BA:2242:G:H2'   | 27:BA:2243:U:O4'  | 2.10                     | 0.51              |
| 27:BA:2362:G:H2'   | 27:BA:2363:C:H5'  | 1.92                     | 0.51              |
| 27:BA:2507:C:O2'   | 27:BA:2508:G:H5'  | 2.09                     | 0.51              |
| 27:BA:244:A:C2     | 27:BA:255:A:C4    | 2.99                     | 0.51              |
| 27:BA:408:G:O2'    | 27:BA:409:C:H5'   | 2.10                     | 0.51              |
| 27:BA:422:A:H2'    | 27:BA:423:A:C8    | 2.45                     | 0.51              |
| 27:BA:721:C:H2'    | 27:BA:722:A:C8    | 2.46                     | 0.51              |
| 27:BA:927:G:H5'    | 27:BA:928:G:OP2   | 2.09                     | 0.51              |
| 30:BD:27:THR:HG21  | 30:BD:83:GLU:HA   | 1.92                     | 0.51              |
| 31:BE:75:VAL:CG1   | 31:BE:76:ARG:H    | 2.21                     | 0.51              |
| 33:BG:166:ASP:O    | 33:BG:169:ALA:N   | 2.44                     | 0.51              |
| 33:BG:57:ALA:HA    | 33:BG:90:LEU:HD11 | 1.93                     | 0.51              |
| 34:BH:142:GLY:O    | 34:BH:145:ALA:HB3 | 2.09                     | 0.51              |
| 34:BH:44:VAL:O     | 34:BH:46:GLU:N    | 2.42                     | 0.51              |
| 34:BH:85:LYS:HE2   | 34:BH:145:ALA:CA  | 2.40                     | 0.51              |
| 35:BI:46:ALA:O     | 35:BI:49:ALA:HB3  | 2.10                     | 0.51              |
| 27:BA:662:G:H5'    | 38:BP:17:LYS:O    | 2.11                     | 0.51              |
| 43:BU:52:ARG:HB3   | 43:BU:52:ARG:CZ   | 2.39                     | 0.51              |
| 47:BY:7:VAL:HG21   | 47:BY:8:LYS:HZ3   | 1.74                     | 0.51              |
| 48:BZ:101:LEU:HB2  | 48:BZ:121:ARG:O   | 2.10                     | 0.51              |
| 48:BZ:138:VAL:HG12 | 48:BZ:139:ASP:N   | 2.20                     | 0.51              |
| 1:CA:1297:C:H1'    | 1:CA:1298:C:H5    | 1.74                     | 0.51              |
| 1:CA:556:C:H2'     | 1:CA:557:G:C8     | 2.42                     | 0.51              |
| 1:CA:565:U:H2'     | 1:CA:566:G:H8     | 1.74                     | 0.51              |
| 1:CA:885:G:H2'     | 1:CA:886:G:C8     | 2.37                     | 0.51              |
| 2:CB:42:ILE:HD11   | 2:CB:202:PRO:HB2  | 1.92                     | 0.51              |
| 2:CB:17:PHE:HB2    | 2:CB:42:ILE:HG22  | 1.92                     | 0.51              |
| 2:CB:97:TRP:CZ3    | 2:CB:98:LEU:O     | 2.63                     | 0.51              |
| 5:CE:45:PHE:CG     | 5:CE:47:LYS:HE3   | 2.45                     | 0.51              |
| 1:CA:538:G:C5'     | 12:CL:111:LYS:HD3 | 2.40                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:CL:15:VAL:O     | 12:CL:16:ARG:CB    | 2.58                     | 0.51              |
| 12:CL:25:LYS:O     | 12:CL:27:ALA:N     | 2.43                     | 0.51              |
| 13:CM:53:VAL:HG12  | 13:CM:54:VAL:N     | 2.24                     | 0.51              |
| 1:CA:473:G:H5''    | 16:CP:81:ARG:NH2   | 2.25                     | 0.51              |
| 17:CQ:7:THR:CG2    | 17:CQ:58:GLU:HG2   | 2.40                     | 0.51              |
| 23:CW:42:G:H8      | 23:CW:42:G:O5'     | 1.92                     | 0.51              |
| 25:CY:48:C:O2'     | 25:CY:49:G:H8      | 1.93                     | 0.51              |
| 25:CY:59:U:O2'     | 25:CY:60:C:H5''    | 2.09                     | 0.51              |
| 52:D3:8:LEU:HD12   | 52:D3:30:ARG:O     | 2.10                     | 0.51              |
| 27:DA:1936:A:C8    | 27:DA:1940:U:O2    | 2.64                     | 0.51              |
| 27:DA:2023:G:O2'   | 27:DA:2024:G:H8    | 1.92                     | 0.51              |
| 27:DA:2367:G:H2'   | 27:DA:2368:C:H6    | 1.74                     | 0.51              |
| 27:DA:2507:C:C2    | 27:DA:2508:G:C8    | 2.99                     | 0.51              |
| 27:DA:292:C:H2'    | 27:DA:293:U:H5'    | 1.92                     | 0.51              |
| 27:DA:845:G:H5''   | 27:DA:845:G:C8     | 2.46                     | 0.51              |
| 27:DA:940:G:C2'    | 27:DA:941:A:H5''   | 2.40                     | 0.51              |
| 28:DB:2:C:H2'      | 28:DB:3:C:C6       | 2.45                     | 0.51              |
| 30:DD:131:LEU:HA   | 30:DD:190:TYR:CE2  | 2.46                     | 0.51              |
| 30:DD:210:GLY:C    | 30:DD:212:SER:H    | 2.13                     | 0.51              |
| 31:DE:116:VAL:O    | 31:DE:116:VAL:HG22 | 2.09                     | 0.51              |
| 31:DE:175:VAL:HG23 | 31:DE:177:PRO:HD3  | 1.91                     | 0.51              |
| 32:DF:65:TRP:CH2   | 32:DF:75:HIS:CD2   | 2.98                     | 0.51              |
| 35:DI:15:VAL:HG23  | 35:DI:16:GLY:N     | 2.24                     | 0.51              |
| 35:DI:81:VAL:HG12  | 35:DI:82:ARG:N     | 2.24                     | 0.51              |
| 37:DO:104:ARG:HH22 | 42:DT:43:GLN:HE22  | 1.58                     | 0.51              |
| 37:DO:105:GLU:N    | 37:DO:105:GLU:OE1  | 2.43                     | 0.51              |
| 37:DO:66:LYS:HD2   | 37:DO:78:ARG:HG3   | 1.91                     | 0.51              |
| 42:DT:134:GLU:O    | 42:DT:135:ALA:HB3  | 2.10                     | 0.51              |
| 44:DV:49:THR:HG22  | 44:DV:50:PRO:CD    | 2.38                     | 0.51              |
| 27:DA:483:A:H1'    | 47:DY:60:PHE:HZ    | 1.75                     | 0.51              |
| 48:DZ:12:GLU:O     | 48:DZ:17:LEU:HD13  | 2.10                     | 0.51              |
| 1:AA:102:G:O2'     | 1:AA:103:C:H5'     | 2.10                     | 0.51              |
| 1:AA:1173:G:H2'    | 1:AA:1174:G:H8     | 1.76                     | 0.51              |
| 1:AA:981:U:O4      | 1:AA:1222:G:O6     | 2.28                     | 0.51              |
| 1:AA:182:U:C6      | 1:AA:182:U:H5'     | 2.44                     | 0.51              |
| 1:AA:275:G:C2'     | 1:AA:276:G:H5'     | 2.41                     | 0.51              |
| 1:AA:505:G:H2'     | 1:AA:506:G:C8      | 2.45                     | 0.51              |
| 1:AA:631:G:C5'     | 1:AA:632:A:OP1     | 2.54                     | 0.51              |
| 1:AA:950:U:H2'     | 1:AA:951:G:C8      | 2.44                     | 0.51              |
| 1:AA:994:A:N7      | 1:AA:1216:G:H4'    | 2.25                     | 0.51              |
| 3:AC:155:GLY:O     | 3:AC:156:ARG:HB2   | 2.10                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AC:164:ARG:O    | 3:AC:165:THR:CB    | 2.59                     | 0.51              |
| 3:AC:201:TYR:CD1  | 3:AC:201:TYR:N     | 2.79                     | 0.51              |
| 4:AD:123:HIS:O    | 4:AD:125:HIS:CG    | 2.63                     | 0.51              |
| 9:AI:112:LYS:HA   | 9:AI:119:ALA:N     | 2.25                     | 0.51              |
| 1:AA:36:C:H4'     | 12:AL:119:THR:O    | 2.10                     | 0.51              |
| 13:AM:64:TRP:CD1  | 13:AM:64:TRP:N     | 2.77                     | 0.51              |
| 24:AX:3:C:O2      | 24:AX:3:C:H2'      | 2.09                     | 0.51              |
| 24:AX:63:G:H2'    | 24:AX:63:G:N3      | 2.25                     | 0.51              |
| 51:B2:6:VAL:HG13  | 51:B2:59:ARG:HH11  | 1.74                     | 0.51              |
| 55:B6:48:VAL:O    | 55:B6:49:HIS:CB    | 2.58                     | 0.51              |
| 57:B8:7:HIS:CE1   | 57:B8:9:GLY:HA3    | 2.45                     | 0.51              |
| 27:BA:1811:G:H2'  | 27:BA:1812:A:H8    | 1.76                     | 0.51              |
| 27:BA:1996:C:H1'  | 27:BA:1997:G:O4'   | 2.10                     | 0.51              |
| 27:BA:2048:G:C8   | 27:BA:2048:G:H5'   | 2.37                     | 0.51              |
| 27:BA:2586:C:H5'  | 27:BA:2586:C:H6    | 1.75                     | 0.51              |
| 27:BA:271(T):C:C2 | 27:BA:271(U):G:C8  | 2.98                     | 0.51              |
| 27:BA:380:U:O2    | 27:BA:381:G:C8     | 2.63                     | 0.51              |
| 27:BA:414:C:H5'   | 27:BA:415:A:OP2    | 2.11                     | 0.51              |
| 27:BA:516:C:O2'   | 27:BA:517:C:H5'    | 2.11                     | 0.51              |
| 28:BB:101:G:H2'   | 28:BB:102:A:O4'    | 2.10                     | 0.51              |
| 29:BC:22:ILE:O    | 29:BC:22:ILE:HG22  | 2.10                     | 0.51              |
| 27:BA:764:A:C6    | 30:BD:209:ALA:HB1  | 2.45                     | 0.51              |
| 30:BD:24:ILE:O    | 30:BD:25:THR:O     | 2.28                     | 0.51              |
| 33:BG:28:VAL:O    | 33:BG:31:VAL:CG1   | 2.58                     | 0.51              |
| 34:BH:157:TYR:O   | 34:BH:158:HIS:CD2  | 2.62                     | 0.51              |
| 38:BP:24:GLY:O    | 38:BP:25:SER:CB    | 2.55                     | 0.51              |
| 40:BR:41:ALA:O    | 40:BR:43:GLU:N     | 2.43                     | 0.51              |
| 43:BU:61:TRP:O    | 43:BU:64:ARG:N     | 2.43                     | 0.51              |
| 47:BY:27:VAL:HA   | 47:BY:28:LYS:HZ1   | 1.67                     | 0.51              |
| 48:BZ:6:ALA:O     | 48:BZ:61:PRO:HD3   | 2.10                     | 0.51              |
| 48:BZ:95:VAL:HG12 | 48:BZ:96:GLU:N     | 2.26                     | 0.51              |
| 1:CA:1030:C:C3'   | 1:CA:1030(A):G:H5' | 2.40                     | 0.51              |
| 1:CA:815:A:O2'    | 1:CA:1527:C:C1'    | 2.59                     | 0.51              |
| 1:CA:44:G:H2'     | 1:CA:45:U:O4'      | 2.11                     | 0.51              |
| 2:CB:200:ILE:HG22 | 2:CB:201:ILE:N     | 2.26                     | 0.51              |
| 3:CC:188:LEU:O    | 3:CC:189:ALA:HB3   | 2.11                     | 0.51              |
| 5:CE:15:ARG:HG3   | 5:CE:28:PHE:HE2    | 1.69                     | 0.51              |
| 5:CE:94:ALA:HB1   | 5:CE:98:THR:CB     | 2.41                     | 0.51              |
| 9:CI:89:ASN:HB3   | 9:CI:92:TYR:HD1    | 1.71                     | 0.51              |
| 12:CL:56:ARG:HG3  | 12:CL:61:TYR:O     | 2.10                     | 0.51              |
| 14:CN:41:ARG:O    | 14:CN:44:LEU:HB3   | 2.10                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:CP:22:THR:HB    | 16:CP:32:TYR:HA   | 1.93                     | 0.51              |
| 19:CS:32:LYS:CE    | 19:CS:32:LYS:H    | 2.17                     | 0.51              |
| 55:D6:15:GLU:HB3   | 55:D6:18:ARG:CG   | 2.40                     | 0.51              |
| 27:DA:1320:C:H5''  | 27:DA:1321:A:OP1  | 2.11                     | 0.51              |
| 27:DA:1340:U:O2'   | 27:DA:1602:U:H2'  | 2.11                     | 0.51              |
| 27:DA:1833:U:H2'   | 27:DA:1834:U:C6   | 2.45                     | 0.51              |
| 27:DA:2283:C:H2'   | 27:DA:2284:C:C5'  | 2.39                     | 0.51              |
| 27:DA:284:U:O2'    | 27:DA:285:C:H6    | 1.92                     | 0.51              |
| 27:DA:321:G:C2     | 32:DF:165:ARG:CZ  | 2.93                     | 0.51              |
| 27:DA:708:C:H42    | 27:DA:723:G:H1    | 1.58                     | 0.51              |
| 28:DB:16:G:H1      | 28:DB:68:C:N4     | 2.05                     | 0.51              |
| 30:DD:45:ASN:HB2   | 30:DD:46:GLN:OE1  | 2.11                     | 0.51              |
| 27:DA:2811:G:C1'   | 31:DE:61:ARG:HH21 | 2.23                     | 0.51              |
| 38:DP:84:ASN:C     | 38:DP:86:LYS:H    | 2.12                     | 0.51              |
| 39:DQ:2:LEU:O      | 39:DQ:70:PRO:HG2  | 2.10                     | 0.51              |
| 44:DV:19:LYS:HZ1   | 44:DV:22:VAL:HG13 | 1.75                     | 0.51              |
| 45:DW:88:ARG:HB2   | 45:DW:92:ARG:CB   | 2.39                     | 0.51              |
| 46:DX:63:LYS:HE3   | 46:DX:72:LYS:HG3  | 1.91                     | 0.51              |
| 46:DX:59:VAL:HG21  | 46:DX:78:LYS:HD2  | 1.92                     | 0.51              |
| 1:AA:477:A:O2'     | 1:AA:479:C:H5'    | 2.10                     | 0.51              |
| 1:AA:494:U:H6      | 1:AA:494:U:O5'    | 1.94                     | 0.51              |
| 3:AC:152:ILE:HG22  | 3:AC:153:VAL:N    | 2.25                     | 0.51              |
| 4:AD:178:VAL:C     | 4:AD:180:GLY:N    | 2.63                     | 0.51              |
| 13:AM:104:ARG:CG   | 13:AM:105:THR:N   | 2.71                     | 0.51              |
| 15:AO:62:GLN:HE21  | 15:AO:66:LEU:HD13 | 1.76                     | 0.51              |
| 20:AT:73:HIS:CG    | 20:AT:74:LYS:H    | 2.29                     | 0.51              |
| 20:AT:78:ALA:HA    | 20:AT:81:LYS:HD3  | 1.92                     | 0.51              |
| 20:AT:90:GLN:O     | 20:AT:91:LEU:HD23 | 2.11                     | 0.51              |
| 54:B5:37:LYS:HG3   | 54:B5:38:ALA:N    | 2.26                     | 0.51              |
| 27:BA:142(A):C:C2' | 27:BA:143:G:H5'   | 2.40                     | 0.51              |
| 27:BA:188:G:C2'    | 27:BA:189:G:H5'   | 2.40                     | 0.51              |
| 27:BA:2159:G:O2'   | 27:BA:2160:G:O5'  | 2.28                     | 0.51              |
| 27:BA:2208:A:H1'   | 27:BA:2219:G:C4   | 2.46                     | 0.51              |
| 27:BA:2271:G:C5    | 27:BA:2272:U:C5   | 2.97                     | 0.51              |
| 27:BA:2817:G:H21   | 27:BA:2836:U:C1'  | 2.24                     | 0.51              |
| 27:BA:377:C:H2'    | 27:BA:378:C:C6    | 2.45                     | 0.51              |
| 27:BA:628:G:H2'    | 27:BA:629:G:C8    | 2.46                     | 0.51              |
| 27:BA:68:G:N2      | 27:BA:74:A:O4'    | 2.43                     | 0.51              |
| 28:BB:43:C:H3'     | 28:BB:44:G:H5'    | 1.92                     | 0.51              |
| 28:BB:47:C:O2'     | 41:BS:93:LYS:HG2  | 2.11                     | 0.51              |
| 29:BC:36:LYS:HB2   | 29:BC:36:LYS:NZ   | 2.24                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BD:197:GLY:O   | 30:BD:198:ASN:CB  | 2.58                     | 0.51              |
| 30:BD:238:GLY:O   | 30:BD:239:ARG:HB3 | 2.10                     | 0.51              |
| 31:BE:86:PRO:C    | 31:BE:88:GLY:N    | 2.64                     | 0.51              |
| 31:BE:36:ARG:HH22 | 31:BE:88:GLY:CA   | 2.19                     | 0.51              |
| 31:BE:9:VAL:CG1   | 31:BE:25:VAL:HG12 | 2.38                     | 0.51              |
| 34:BH:89:ILE:HG12 | 34:BH:129:THR:HA  | 1.91                     | 0.51              |
| 34:BH:85:LYS:HZ2  | 34:BH:133:VAL:CG2 | 2.23                     | 0.51              |
| 36:BN:17:ASP:HB2  | 36:BN:55:VAL:HG12 | 1.89                     | 0.51              |
| 36:BN:55:VAL:HG22 | 36:BN:56:ASN:N    | 2.26                     | 0.51              |
| 38:BP:8:PRO:O     | 38:BP:9:ASN:HB3   | 2.10                     | 0.51              |
| 40:BR:79:LEU:HA   | 40:BR:83:ILE:HB   | 1.92                     | 0.51              |
| 42:BT:129:ARG:NH1 | 42:BT:131:ALA:N   | 2.58                     | 0.51              |
| 43:BU:66:ASN:CB   | 43:BU:76:TYR:HB2  | 2.40                     | 0.51              |
| 44:BV:19:LYS:HB2  | 44:BV:96:ILE:HG12 | 1.91                     | 0.51              |
| 27:BA:2013:A:H4'  | 45:BW:96:ILE:HD12 | 1.91                     | 0.51              |
| 48:BZ:9:ARG:NH2   | 48:BZ:25:GLY:O    | 2.44                     | 0.51              |
| 1:CA:1026:G:H5'   | 1:CA:1027:C:OP2   | 2.11                     | 0.51              |
| 1:CA:1095:U:N3    | 1:CA:1096:C:C4    | 2.78                     | 0.51              |
| 1:CA:1368:G:H5''  | 9:CI:112:LYS:HG2  | 1.92                     | 0.51              |
| 1:CA:1398:A:C5'   | 1:CA:1398:A:C8    | 2.92                     | 0.51              |
| 1:CA:1441:G:H5''  | 1:CA:1442:G:O4'   | 2.11                     | 0.51              |
| 1:CA:1445:C:H2'   | 1:CA:1446:U:C5'   | 2.40                     | 0.51              |
| 1:CA:224:C:O2'    | 1:CA:225:C:H5'    | 2.11                     | 0.51              |
| 1:CA:841:U:H3'    | 1:CA:848:C:O4'    | 2.10                     | 0.51              |
| 1:CA:992:U:H4'    | 1:CA:993:G:C5'    | 2.39                     | 0.51              |
| 2:CB:14:GLY:C     | 2:CB:15:VAL:HG22  | 2.31                     | 0.51              |
| 3:CC:142:MET:C    | 3:CC:144:SER:H    | 2.14                     | 0.51              |
| 3:CC:23:TYR:CG    | 3:CC:24:ALA:N     | 2.78                     | 0.51              |
| 3:CC:6:HIS:O      | 3:CC:8:ILE:N      | 2.43                     | 0.51              |
| 3:CC:72:LYS:N     | 3:CC:73:PRO:CD    | 2.73                     | 0.51              |
| 6:CF:6:VAL:HG22   | 6:CF:90:VAL:CG1   | 2.40                     | 0.51              |
| 7:CG:24:THR:C     | 7:CG:28:ASN:HD22  | 2.14                     | 0.51              |
| 10:CJ:82:ILE:HA   | 10:CJ:85:LEU:HD12 | 1.92                     | 0.51              |
| 12:CL:24:LEU:HD13 | 12:CL:24:LEU:N    | 2.25                     | 0.51              |
| 15:CO:79:ARG:HA   | 15:CO:82:ILE:CG2  | 2.41                     | 0.51              |
| 16:CP:58:TYR:C    | 16:CP:60:LEU:H    | 2.13                     | 0.51              |
| 19:CS:6:LYS:HE3   | 19:CS:6:LYS:N     | 2.25                     | 0.51              |
| 24:CX:17:C:H5''   | 24:CX:17(B):U:H2' | 1.92                     | 0.51              |
| 51:D2:2:LYS:N     | 51:D2:5:GLU:OE1   | 2.43                     | 0.51              |
| 58:D9:17:ILE:CG2  | 58:D9:19:ARG:HG2  | 2.39                     | 0.51              |
| 27:DA:1435:G:H2'  | 27:DA:1436:G:O4'  | 2.09                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:1814:G:H2'  | 27:DA:1815:A:C8   | 2.45                     | 0.51              |
| 27:DA:2197:U:O2'  | 27:DA:2198:A:P    | 2.68                     | 0.51              |
| 27:DA:2402:C:H2'  | 27:DA:2403:C:O5'  | 2.11                     | 0.51              |
| 27:DA:2500:U:C2'  | 27:DA:2504:U:H5   | 2.24                     | 0.51              |
| 27:DA:252:G:H2'   | 27:DA:253:C:H6    | 1.75                     | 0.51              |
| 27:DA:2721:A:H2'  | 27:DA:2722:G:O4'  | 2.10                     | 0.51              |
| 27:DA:2751:G:H3'  | 27:DA:2752:C:H5   | 1.74                     | 0.51              |
| 29:DC:78:ALA:CB   | 29:DC:82:LYS:HD2  | 2.40                     | 0.51              |
| 30:DD:25:THR:O    | 30:DD:26:LYS:C    | 2.49                     | 0.51              |
| 34:DH:93:GLY:C    | 34:DH:94:TYR:HD1  | 2.14                     | 0.51              |
| 35:DI:73:GLU:OE2  | 35:DI:137:PRO:HD2 | 2.11                     | 0.51              |
| 37:DO:40:VAL:HG12 | 37:DO:41:ALA:N    | 2.26                     | 0.51              |
| 38:DP:101:VAL:C   | 38:DP:103:ALA:H   | 2.13                     | 0.51              |
| 39:DQ:110:THR:CG2 | 39:DQ:113:GLN:HB2 | 2.40                     | 0.51              |
| 41:DS:22:GLY:O    | 41:DS:23:ARG:O    | 2.27                     | 0.51              |
| 41:DS:36:TYR:N    | 41:DS:36:TYR:CD1  | 2.78                     | 0.51              |
| 47:DY:95:LYS:HG2  | 47:DY:100:ALA:HA  | 1.93                     | 0.51              |
| 47:DY:20:TYR:CZ   | 47:DY:42:VAL:HA   | 2.46                     | 0.51              |
| 1:AA:1049:U:H4'   | 1:AA:1050:G:OP2   | 2.10                     | 0.51              |
| 1:AA:1203:C:H2'   | 1:AA:1204:A:C8    | 2.43                     | 0.51              |
| 1:AA:1245:A:H61   | 1:AA:1292:U:H3    | 1.57                     | 0.51              |
| 1:AA:1305:G:N2    | 1:AA:1331:G:C2'   | 2.68                     | 0.51              |
| 1:AA:1371:G:O2'   | 1:AA:1372:U:H5'   | 2.11                     | 0.51              |
| 1:AA:547:A:H5'    | 1:AA:548:G:OP1    | 2.11                     | 0.51              |
| 1:AA:865:A:H5'    | 1:AA:1078:U:C4    | 2.45                     | 0.51              |
| 2:AB:110:GLN:HA   | 2:AB:113:HIS:HB2  | 1.92                     | 0.51              |
| 2:AB:16:HIS:CD2   | 2:AB:210:SER:HA   | 2.46                     | 0.51              |
| 3:AC:86:VAL:O     | 3:AC:90:GLU:HG2   | 2.11                     | 0.51              |
| 5:AE:127:ASN:O    | 5:AE:131:ILE:HG12 | 2.11                     | 0.51              |
| 6:AF:8:ILE:HG12   | 6:AF:88:VAL:HG22  | 1.93                     | 0.51              |
| 9:AI:120:ARG:O    | 9:AI:121:ARG:C    | 2.48                     | 0.51              |
| 12:AL:10:LYS:HD2  | 12:AL:10:LYS:H    | 1.71                     | 0.51              |
| 13:AM:83:ASP:C    | 13:AM:85:GLY:H    | 2.13                     | 0.51              |
| 13:AM:91:ARG:HD3  | 19:AS:81:ARG:HH21 | 1.76                     | 0.51              |
| 49:B0:45:PHE:CZ   | 49:B0:77:ARG:NH2  | 2.79                     | 0.51              |
| 51:B2:33:MET:C    | 51:B2:35:LEU:N    | 2.60                     | 0.51              |
| 53:B4:40:ILE:N    | 53:B4:40:ILE:HD12 | 2.26                     | 0.51              |
| 56:B7:37:LYS:HD3  | 56:B7:39:ARG:CD   | 2.40                     | 0.51              |
| 27:BA:1659:U:O2'  | 27:BA:1660:C:H5'  | 2.11                     | 0.51              |
| 27:BA:2164:C:H2'  | 27:BA:2165:G:O4'  | 2.10                     | 0.51              |
| 27:BA:438:G:H2'   | 27:BA:440:G:H8    | 1.76                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:481:G:C1'   | 27:BA:506:G:N2     | 2.72                     | 0.51              |
| 27:BA:536:A:H2'   | 27:BA:537:C:H6     | 1.73                     | 0.51              |
| 27:BA:744:G:C6    | 27:BA:745:G:C4     | 2.98                     | 0.51              |
| 27:BA:2121:G:H21  | 29:BC:172:HIS:CB   | 2.23                     | 0.51              |
| 29:BC:56:GLN:NE2  | 29:BC:173:ALA:HB1  | 2.26                     | 0.51              |
| 30:BD:270:ILE:C   | 30:BD:271:ILE:HG12 | 2.30                     | 0.51              |
| 31:BE:81:ILE:HG21 | 31:BE:84:PHE:CD1   | 2.45                     | 0.51              |
| 33:BG:33:ARG:O    | 33:BG:161:THR:HG22 | 2.10                     | 0.51              |
| 27:BA:2305:A:N6   | 33:BG:43:LEU:H     | 2.06                     | 0.51              |
| 36:BN:28:THR:HG23 | 36:BN:29:LYS:N     | 2.25                     | 0.51              |
| 36:BN:53:VAL:O    | 36:BN:54:VAL:C     | 2.49                     | 0.51              |
| 38:BP:63:PRO:O    | 38:BP:65:ARG:N     | 2.44                     | 0.51              |
| 39:BQ:41:TRP:C    | 39:BQ:42:ILE:HD12  | 2.31                     | 0.51              |
| 41:BS:96:GLY:O    | 41:BS:98:VAL:HG12  | 2.10                     | 0.51              |
| 47:BY:2:ARG:O     | 47:BY:4:LYS:N      | 2.44                     | 0.51              |
| 47:BY:7:VAL:CB    | 47:BY:8:LYS:NZ     | 2.72                     | 0.51              |
| 48:BZ:152:SER:CB  | 48:BZ:166:PRO:HB3  | 2.40                     | 0.51              |
| 48:BZ:44:ASP:O    | 48:BZ:45:LYS:C     | 2.49                     | 0.51              |
| 1:CA:1014:A:H2'   | 1:CA:1015:A:N9     | 2.25                     | 0.51              |
| 1:CA:1101:A:C4'   | 1:CA:1102:A:O5'    | 2.35                     | 0.51              |
| 1:CA:1161:C:H42   | 1:CA:1176:A:H61    | 1.59                     | 0.51              |
| 1:CA:1440:C:O2    | 1:CA:1440:C:H2'    | 2.10                     | 0.51              |
| 1:CA:1492:A:H5'   | 26:CZ:6:5OH:CB     | 2.40                     | 0.51              |
| 1:CA:1505:G:H4'   | 1:CA:1506:U:H5'    | 1.93                     | 0.51              |
| 1:CA:237:C:O2'    | 1:CA:238:G:H5'     | 2.10                     | 0.51              |
| 1:CA:502:G:OP1    | 12:CL:115:SER:N    | 2.44                     | 0.51              |
| 1:CA:607:A:H2'    | 1:CA:608:A:H5'     | 1.93                     | 0.51              |
| 1:CA:741:G:H2'    | 1:CA:742:G:H8      | 1.75                     | 0.51              |
| 1:CA:859:A:H2'    | 1:CA:860:A:C5'     | 2.40                     | 0.51              |
| 1:CA:859:A:H2'    | 1:CA:860:A:H5'     | 1.91                     | 0.51              |
| 1:CA:985:C:O2'    | 1:CA:986:A:C8      | 2.59                     | 0.51              |
| 4:CD:25:ARG:NH1   | 4:CD:30:LYS:O      | 2.44                     | 0.51              |
| 5:CE:47:LYS:O     | 5:CE:48:ALA:HB2    | 2.10                     | 0.51              |
| 5:CE:79:GLU:HA    | 5:CE:91:LEU:O      | 2.10                     | 0.51              |
| 7:CG:111:ARG:HB3  | 7:CG:111:ARG:NH1   | 2.25                     | 0.51              |
| 10:CJ:33:GLN:OE1  | 10:CJ:75:ILE:HD11  | 2.10                     | 0.51              |
| 10:CJ:87:THR:OG1  | 10:CJ:88:LEU:N     | 2.42                     | 0.51              |
| 13:CM:106:ASN:O   | 13:CM:107:ALA:HB3  | 2.10                     | 0.51              |
| 13:CM:12:ASN:OD1  | 13:CM:46:LYS:HE2   | 2.10                     | 0.51              |
| 52:D3:49:LYS:HG2  | 52:D3:49:LYS:O     | 2.11                     | 0.51              |
| 54:D5:57:VAL:HG23 | 54:D5:58:LEU:N     | 2.26                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 54:D5:8:LYS:O      | 54:D5:9:LYS:HG2   | 2.11                     | 0.51              |
| 27:DA:1339:G:N2    | 27:DA:1603:A:H1'  | 2.25                     | 0.51              |
| 27:DA:1817:G:H2'   | 27:DA:1818:U:H5'  | 1.93                     | 0.51              |
| 27:DA:1932:A:C2'   | 27:DA:1933:G:H5'  | 2.41                     | 0.51              |
| 27:DA:1935:G:C6    | 27:DA:1962:C:C6   | 2.99                     | 0.51              |
| 27:DA:1980:G:O2'   | 27:DA:1982:C:OP2  | 2.27                     | 0.51              |
| 27:DA:2258:C:C4'   | 27:DA:2259:G:OP2  | 2.57                     | 0.51              |
| 27:DA:2580:U:H5'   | 27:DA:2581:G:OP2  | 2.10                     | 0.51              |
| 27:DA:2656:U:HO2'  | 27:DA:2657:A:H8   | 1.59                     | 0.51              |
| 27:DA:2672:G:C3'   | 27:DA:2673:G:H5'' | 2.41                     | 0.51              |
| 27:DA:272(G):C:N4  | 27:DA:363(C):G:H1 | 2.08                     | 0.51              |
| 27:DA:363(D):G:H2' | 27:DA:363(D):G:N3 | 2.26                     | 0.51              |
| 27:DA:76:C:O5'     | 27:DA:76:C:H6     | 1.93                     | 0.51              |
| 30:DD:176:ARG:HG2  | 30:DD:177:LEU:N   | 2.26                     | 0.51              |
| 27:DA:773:U:H4'    | 30:DD:47:GLY:HA3  | 1.93                     | 0.51              |
| 31:DE:52:LEU:HD23  | 31:DE:76:ARG:HB2  | 1.92                     | 0.51              |
| 34:DH:12:PRO:HG2   | 34:DH:49:VAL:CA   | 2.30                     | 0.51              |
| 34:DH:74:ASN:N     | 34:DH:74:ASN:HD22 | 2.09                     | 0.51              |
| 35:DI:26:ALA:HB1   | 35:DI:31:LEU:CD1  | 2.41                     | 0.51              |
| 27:DA:1654:A:OP1   | 40:DR:3:HIS:HB2   | 2.09                     | 0.51              |
| 40:DR:93:GLY:C     | 40:DR:95:THR:H    | 2.14                     | 0.51              |
| 43:DU:49:HIS:CA    | 43:DU:52:ARG:HB2  | 2.33                     | 0.51              |
| 27:DA:536:A:OP1    | 43:DU:53:ARG:NH1  | 2.44                     | 0.51              |
| 1:AA:815:A:O2'     | 1:AA:816:A:P      | 2.69                     | 0.51              |
| 8:AH:109:ILE:HD11  | 8:AH:120:THR:CG2  | 2.41                     | 0.51              |
| 1:AA:1350:A:OP2    | 9:AI:118:LYS:HE3  | 2.11                     | 0.51              |
| 11:AK:34:ASP:HB2   | 11:AK:35:PRO:HD2  | 1.91                     | 0.51              |
| 12:AL:25:LYS:HB2   | 12:AL:30:ARG:NH1  | 2.20                     | 0.51              |
| 13:AM:3:ARG:CZ     | 13:AM:7:VAL:HG13  | 2.40                     | 0.51              |
| 19:AS:19:VAL:HG11  | 19:AS:44:MET:HG3  | 1.93                     | 0.51              |
| 25:AY:62:U:H2'     | 25:AY:63:C:C6     | 2.46                     | 0.51              |
| 49:B0:25:ARG:NH1   | 49:B0:25:ARG:HG2  | 2.25                     | 0.51              |
| 27:BA:150:C:O2'    | 27:BA:151:C:H5'   | 2.11                     | 0.51              |
| 27:BA:15:G:H2'     | 27:BA:16:G:C8     | 2.44                     | 0.51              |
| 27:BA:2070:G:N2    | 27:BA:2071:A:N3   | 2.59                     | 0.51              |
| 27:BA:2172:U:C1'   | 27:BA:2173:A:OP1  | 2.52                     | 0.51              |
| 27:BA:229:A:C8     | 27:BA:229:A:OP1   | 2.64                     | 0.51              |
| 27:BA:2481:G:O2'   | 27:BA:2482:G:OP2  | 2.28                     | 0.51              |
| 27:BA:2571:C:C5'   | 27:BA:2572:A:C5'  | 2.79                     | 0.51              |
| 27:BA:598:G:H2'    | 27:BA:599:G:O4'   | 2.10                     | 0.51              |
| 27:BA:796:C:H2'    | 27:BA:797:C:C6    | 2.45                     | 0.51              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 27:BA:6:A:H2      | 27:BA:7:G:C4        | 2.28                     | 0.51              |
| 27:BA:813:U:H2'   | 27:BA:814:C:C6      | 2.46                     | 0.51              |
| 27:BA:876:C:H2'   | 27:BA:877:U:H6      | 1.76                     | 0.51              |
| 31:BE:69:LYS:O    | 31:BE:71:GLY:N      | 2.43                     | 0.51              |
| 36:BN:93:THR:CG2  | 36:BN:93:THR:O      | 2.56                     | 0.51              |
| 39:BQ:37:LEU:HD21 | 39:BQ:130:LYS:HB2   | 1.92                     | 0.51              |
| 41:BS:96:GLY:O    | 41:BS:98:VAL:N      | 2.44                     | 0.51              |
| 43:BU:92:ARG:HH21 | 44:BV:11:GLN:N      | 2.07                     | 0.51              |
| 43:BU:47:TYR:CE2  | 44:BV:74:LYS:NZ     | 2.79                     | 0.51              |
| 47:BY:37:VAL:O    | 47:BY:38:ILE:HG12   | 2.11                     | 0.51              |
| 48:BZ:71:ARG:HE   | 48:BZ:88:PHE:HD1    | 1.59                     | 0.51              |
| 1:CA:1452:C:H1'   | 1:CA:1456:G:N2      | 2.25                     | 0.51              |
| 1:CA:229:U:O2'    | 1:CA:230:G:H5'      | 2.10                     | 0.51              |
| 1:CA:63:C:O2'     | 1:CA:380:G:H4'      | 2.10                     | 0.51              |
| 1:CA:571:U:H3'    | 1:CA:572:A:C5'      | 2.40                     | 0.51              |
| 1:CA:896:C:C2'    | 1:CA:897:C:H5'      | 2.40                     | 0.51              |
| 1:CA:969:A:H2'    | 1:CA:970:C:O4'      | 2.11                     | 0.51              |
| 1:CA:992:U:C4'    | 1:CA:993:G:O5'      | 2.48                     | 0.51              |
| 1:CA:1074:G:C1'   | 2:CB:104:ASN:HD22   | 2.24                     | 0.51              |
| 2:CB:142:LEU:CD1  | 2:CB:146:GLN:HB2    | 2.41                     | 0.51              |
| 2:CB:74:LYS:HD3   | 2:CB:165:VAL:HG21   | 1.93                     | 0.51              |
| 4:CD:33:MET:HE1   | 4:CD:37:PRO:HA      | 1.93                     | 0.51              |
| 4:CD:61:LYS:HZ2   | 4:CD:62:GLN:HE21    | 1.59                     | 0.51              |
| 4:CD:80:GLU:HA    | 4:CD:80:GLU:OE2     | 2.10                     | 0.51              |
| 7:CG:146:GLU:O    | 7:CG:149:ARG:HB2    | 2.10                     | 0.51              |
| 7:CG:48:LYS:O     | 7:CG:52:GLU:HB2     | 2.10                     | 0.51              |
| 12:CL:5:ASN:HA    | 12:CL:8:VAL:HG23    | 1.93                     | 0.51              |
| 14:CN:22:THR:OG1  | 14:CN:33:VAL:CG2    | 2.58                     | 0.51              |
| 52:D3:54:VAL:CG1  | 52:D3:55:ARG:N      | 2.73                     | 0.51              |
| 27:DA:139:G:H2'   | 27:DA:139(A):G:H5'' | 1.92                     | 0.51              |
| 27:DA:1433:U:O2   | 27:DA:1433:U:H2'    | 2.09                     | 0.51              |
| 27:DA:2061:G:N7   | 27:DA:2501:C:H1'    | 2.26                     | 0.51              |
| 27:DA:2306:C:H5   | 27:DA:2307:G:HO2'   | 1.56                     | 0.51              |
| 27:DA:2314:C:H2'  | 27:DA:2315:G:C8     | 2.46                     | 0.51              |
| 27:DA:2318:G:O2'  | 27:DA:2319:G:OP1    | 2.26                     | 0.51              |
| 27:DA:630:G:N2    | 27:DA:633:A:OP2     | 2.44                     | 0.51              |
| 27:DA:671:C:C5    | 38:DP:36:LYS:HE2    | 2.45                     | 0.51              |
| 27:DA:857:C:P     | 49:D0:77:ARG:NH2    | 2.83                     | 0.51              |
| 27:DA:966:G:H2'   | 27:DA:967:C:H6      | 1.75                     | 0.51              |
| 29:DC:52:ARG:NH2  | 29:DC:53:ARG:NH2    | 2.58                     | 0.51              |
| 30:DD:11:PRO:O    | 30:DD:12:SER:C      | 2.49                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DG:46:ALA:O    | 33:DG:82:LEU:HD11 | 2.09                     | 0.51              |
| 34:DH:45:VAL:HG12 | 34:DH:45:VAL:O    | 2.11                     | 0.51              |
| 41:DS:85:VAL:O    | 41:DS:106:ARG:HG3 | 2.10                     | 0.51              |
| 43:DU:113:ALA:C   | 43:DU:115:ALA:H   | 2.13                     | 0.51              |
| 27:DA:2019:A:O3'  | 43:DU:27:LEU:HD12 | 2.11                     | 0.51              |
| 43:DU:69:CYS:HG   | 43:DU:79:PHE:HD1  | 1.58                     | 0.51              |
| 43:DU:65:ILE:CD1  | 43:DU:96:ALA:CB   | 2.89                     | 0.51              |
| 46:DX:12:VAL:O    | 46:DX:13:LEU:HB2  | 2.10                     | 0.51              |
| 46:DX:36:LYS:HG2  | 46:DX:56:THR:HG23 | 1.91                     | 0.51              |
| 48:DZ:13:LYS:N    | 48:DZ:14:PRO:CD   | 2.74                     | 0.51              |
| 1:AA:1264:C:C6    | 1:AA:1264:C:H3'   | 2.44                     | 0.51              |
| 1:AA:1306:A:H2'   | 1:AA:1307:U:H6    | 1.75                     | 0.51              |
| 1:AA:1435:G:H2'   | 1:AA:1436:U:C6    | 2.45                     | 0.51              |
| 1:AA:266:G:H5'    | 1:AA:266:G:C8     | 2.46                     | 0.51              |
| 1:AA:495:A:HO2'   | 1:AA:496:A:P      | 2.33                     | 0.51              |
| 1:AA:610:G:O2'    | 1:AA:611:A:H5'    | 2.09                     | 0.51              |
| 4:AD:64:LEU:HB2   | 4:AD:198:VAL:HG11 | 1.93                     | 0.51              |
| 7:AG:63:LYS:NZ    | 7:AG:67:GLU:HB2   | 2.24                     | 0.51              |
| 8:AH:94:TYR:HE1   | 8:AH:132:GLU:HB2  | 1.76                     | 0.51              |
| 8:AH:86:ILE:CG1   | 8:AH:135:CYS:HA   | 2.40                     | 0.51              |
| 8:AH:2:LEU:HD22   | 8:AH:3:THR:H      | 1.76                     | 0.51              |
| 10:AJ:16:LEU:HD11 | 10:AJ:70:ARG:NE   | 2.26                     | 0.51              |
| 10:AJ:49:VAL:CG2  | 10:AJ:50:ILE:N    | 2.73                     | 0.51              |
| 11:AK:48:ILE:CG1  | 11:AK:64:ALA:HA   | 2.41                     | 0.51              |
| 13:AM:3:ARG:HG2   | 13:AM:9:ILE:HG13  | 1.92                     | 0.51              |
| 14:AN:24:CYS:N    | 14:AN:33:VAL:HG11 | 2.26                     | 0.51              |
| 15:AO:81:LEU:O    | 15:AO:84:LYS:HD3  | 2.11                     | 0.51              |
| 1:AA:376:G:C5'    | 16:AP:5:ARG:HB2   | 2.27                     | 0.51              |
| 50:B1:93:GLU:C    | 50:B1:95:LEU:N    | 2.62                     | 0.51              |
| 55:B6:9:LEU:HD13  | 55:B6:28:ARG:HG3  | 1.93                     | 0.51              |
| 27:BA:104:U:C6    | 27:BA:105:C:C6    | 2.99                     | 0.51              |
| 27:BA:1164:G:H2'  | 27:BA:1165:U:C6   | 2.46                     | 0.51              |
| 27:BA:1439:A:C2   | 27:BA:1553:A:C5   | 2.98                     | 0.51              |
| 27:BA:1625:C:H2'  | 27:BA:1626:G:H5'  | 1.92                     | 0.51              |
| 27:BA:2362:G:C2'  | 27:BA:2363:C:H5'  | 2.40                     | 0.51              |
| 27:BA:2580:U:H5'  | 31:BE:131:ALA:H   | 1.74                     | 0.51              |
| 27:BA:2590:A:O2'  | 27:BA:2591:C:H5'  | 2.11                     | 0.51              |
| 27:BA:2765:A:H5'  | 27:BA:2766:G:OP2  | 2.10                     | 0.51              |
| 27:BA:2853:C:H2'  | 27:BA:2854:G:H8   | 1.72                     | 0.51              |
| 27:BA:2862:G:O2'  | 27:BA:2863:C:H5'  | 2.11                     | 0.51              |
| 27:BA:382:G:O2'   | 27:BA:383:U:H5'   | 2.10                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:521:G:H2'    | 27:BA:522:G:C8     | 2.45                     | 0.51              |
| 27:BA:703:U:H2'    | 27:BA:704:G:C5'    | 2.40                     | 0.51              |
| 27:BA:826:U:C4     | 27:BA:828:U:H1'    | 2.46                     | 0.51              |
| 28:BB:43:C:H3'     | 28:BB:44:G:C5'     | 2.40                     | 0.51              |
| 29:BC:68:LEU:HD11  | 29:BC:180:PHE:CB   | 2.40                     | 0.51              |
| 27:BA:1843:C:O2'   | 30:BD:256:GLY:HA3  | 2.11                     | 0.51              |
| 31:BE:105:THR:HG21 | 31:BE:164:ARG:HH11 | 1.76                     | 0.51              |
| 31:BE:119:ARG:CD   | 31:BE:120:TRP:CE2  | 2.93                     | 0.51              |
| 31:BE:167:VAL:CG1  | 31:BE:189:PRO:HD3  | 2.41                     | 0.51              |
| 32:BF:10:PRO:HA    | 32:BF:127:GLU:HB3  | 1.93                     | 0.51              |
| 32:BF:186:ILE:HD13 | 32:BF:192:LEU:HD11 | 1.93                     | 0.51              |
| 34:BH:12:PRO:O     | 34:BH:13:LYS:HB2   | 2.09                     | 0.51              |
| 36:BN:18:ALA:HB1   | 36:BN:21:LYS:CB    | 2.40                     | 0.51              |
| 36:BN:63:THR:O     | 36:BN:64:GLY:C     | 2.49                     | 0.51              |
| 38:BP:71:VAL:HG13  | 38:BP:72:PRO:CD    | 2.41                     | 0.51              |
| 39:BQ:37:LEU:HD23  | 39:BQ:129:THR:HA   | 1.93                     | 0.51              |
| 27:BA:2873:A:C2    | 40:BR:6:SER:CB     | 2.93                     | 0.51              |
| 40:BR:73:VAL:O     | 40:BR:76:VAL:HG12  | 2.11                     | 0.51              |
| 42:BT:112:ARG:O    | 42:BT:115:ARG:HG2  | 2.11                     | 0.51              |
| 48:BZ:107:PRO:CG   | 48:BZ:116:LEU:HB2  | 2.40                     | 0.51              |
| 1:CA:1349:A:OP2    | 9:CI:118:LYS:NZ    | 2.43                     | 0.51              |
| 1:CA:257:G:C2      | 1:CA:270:A:N1      | 2.79                     | 0.51              |
| 1:CA:277:C:P       | 17:CQ:41:LYS:HZ2   | 2.34                     | 0.51              |
| 1:CA:576:G:H3'     | 1:CA:577:G:H5''    | 1.93                     | 0.51              |
| 1:CA:876:G:O5'     | 8:CH:14:ARG:NH1    | 2.43                     | 0.51              |
| 1:CA:893:C:H2'     | 1:CA:894:G:C8      | 2.44                     | 0.51              |
| 4:CD:3:ARG:HG2     | 4:CD:118:ARG:CD    | 2.41                     | 0.51              |
| 8:CH:72:PRO:O      | 8:CH:73:ASP:CB     | 2.58                     | 0.51              |
| 11:CK:110:ASP:O    | 18:CR:84:LYS:CG    | 2.59                     | 0.51              |
| 12:CL:79:VAL:HB    | 12:CL:103:ASP:OD1  | 2.11                     | 0.51              |
| 15:CO:54:ARG:O     | 15:CO:54:ARG:HD2   | 2.10                     | 0.51              |
| 18:CR:59:SER:H     | 18:CR:62:GLU:HB2   | 1.76                     | 0.51              |
| 19:CS:22:LEU:HD13  | 19:CS:27:GLU:HB3   | 1.92                     | 0.51              |
| 51:D2:5:GLU:O      | 51:D2:8:LYS:N      | 2.37                     | 0.51              |
| 27:DA:126:A:OP2    | 56:D7:19:ARG:CB    | 2.58                     | 0.51              |
| 27:DA:1877:A:H3'   | 27:DA:1878:G:O4'   | 2.10                     | 0.51              |
| 27:DA:1903:G:N2    | 27:DA:1904:G:C4    | 2.78                     | 0.51              |
| 27:DA:226:G:O2'    | 27:DA:227:A:C8     | 2.53                     | 0.51              |
| 27:DA:2470:G:H2'   | 27:DA:2471:C:H6    | 1.75                     | 0.51              |
| 27:DA:194:G:N2     | 27:DA:251:A:C2     | 2.79                     | 0.51              |
| 27:DA:2650:U:H2'   | 27:DA:2651:C:H6    | 1.76                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:2841:C:H2'  | 27:DA:2842:G:C8    | 2.46                     | 0.51              |
| 29:DC:47:LEU:CB   | 29:DC:207:THR:HA   | 2.40                     | 0.51              |
| 32:DF:41:LEU:HD11 | 32:DF:184:TYR:HE1  | 1.74                     | 0.51              |
| 33:DG:137:GLU:HA  | 33:DG:152:LEU:HD11 | 1.92                     | 0.51              |
| 34:DH:108:GLY:O   | 34:DH:109:PHE:O    | 2.29                     | 0.51              |
| 36:DN:2:LYS:NZ    | 44:DV:13:ARG:N     | 2.55                     | 0.51              |
| 38:DP:112:LEU:C   | 38:DP:112:LEU:HD13 | 2.31                     | 0.51              |
| 47:DY:45:VAL:HG12 | 47:DY:46:LYS:N     | 2.24                     | 0.51              |
| 48:DZ:29:ASN:O    | 48:DZ:30:ARG:HB2   | 2.11                     | 0.51              |
| 1:AA:1090:U:O2'   | 1:AA:1091:U:H5'    | 2.10                     | 0.51              |
| 1:AA:1221:G:P     | 19:AS:36:ARG:HD3   | 2.51                     | 0.51              |
| 1:AA:686:U:O2'    | 1:AA:687:A:H8      | 1.94                     | 0.51              |
| 3:AC:11:ARG:HA    | 3:AC:14:ILE:CG2    | 2.41                     | 0.51              |
| 3:AC:99:VAL:HG23  | 3:AC:99:VAL:O      | 2.11                     | 0.51              |
| 4:AD:145:GLU:O    | 4:AD:147:ALA:N     | 2.43                     | 0.51              |
| 4:AD:205:GLU:C    | 4:AD:207:TYR:N     | 2.65                     | 0.51              |
| 4:AD:94:LEU:O     | 4:AD:97:LEU:N      | 2.44                     | 0.51              |
| 8:AH:20:TYR:CA    | 8:AH:65:TYR:HE2    | 2.17                     | 0.51              |
| 2:AB:178:ARG:NH2  | 8:AH:68:ARG:HH22   | 2.09                     | 0.51              |
| 10:AJ:3:LYS:HB2   | 10:AJ:77:PRO:HG3   | 1.92                     | 0.51              |
| 12:AL:54:LYS:HA   | 12:AL:64:THR:HA    | 1.93                     | 0.51              |
| 14:AN:45:ARG:HA   | 14:AN:48:ALA:HB3   | 1.93                     | 0.51              |
| 18:AR:87:ARG:HG2  | 18:AR:87:ARG:HH11  | 1.76                     | 0.51              |
| 19:AS:6:LYS:O     | 19:AS:7:LYS:HD3    | 2.11                     | 0.51              |
| 21:AU:6:ARG:O     | 21:AU:12:LYS:HE2   | 2.11                     | 0.51              |
| 24:AX:31:G:C2     | 24:AX:40:C:C2      | 2.99                     | 0.51              |
| 50:B1:19:GLN:HE21 | 50:B1:19:GLN:CA    | 2.23                     | 0.51              |
| 50:B1:5:CYS:SG    | 50:B1:8:SER:N      | 2.81                     | 0.51              |
| 51:B2:31:GLU:O    | 51:B2:35:LEU:HD12  | 2.11                     | 0.51              |
| 53:B4:62:CYS:SG   | 53:B4:64:LYS:CG    | 2.99                     | 0.51              |
| 54:B5:40:LYS:HD3  | 54:B5:41:PRO:O     | 2.11                     | 0.51              |
| 57:B8:31:HIS:C    | 57:B8:33:ASN:HD22  | 2.13                     | 0.51              |
| 57:B8:34:TRP:CZ2  | 57:B8:35:GLN:HB3   | 2.45                     | 0.51              |
| 58:B9:32:HIS:O    | 58:B9:34:GLN:CG    | 2.59                     | 0.51              |
| 27:BA:1195:G:C2'  | 27:BA:1196:C:H5'   | 2.40                     | 0.51              |
| 27:BA:1210:A:H5'' | 27:BA:1211:U:H2'   | 1.92                     | 0.51              |
| 27:BA:142:A:H1'   | 27:BA:1408:C:C1'   | 2.41                     | 0.51              |
| 27:BA:2109:U:H6   | 27:BA:2109:U:O5'   | 1.94                     | 0.51              |
| 27:BA:2870:C:O2'  | 27:BA:2871:C:H5'   | 2.10                     | 0.51              |
| 27:BA:486:C:H4'   | 45:BW:60:ASN:OD1   | 2.11                     | 0.51              |
| 27:BA:663:G:H2'   | 27:BA:664:C:C6     | 2.45                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:950:G:C6     | 27:BA:951:C:N3     | 2.79                     | 0.51              |
| 31:BE:4:ILE:HD13   | 31:BE:91:VAL:HG12  | 1.92                     | 0.51              |
| 32:BF:132:VAL:HG22 | 32:BF:133:ASN:N    | 2.26                     | 0.51              |
| 34:BH:88:LEU:HD12  | 34:BH:130:ARG:HG3  | 1.93                     | 0.51              |
| 35:BI:31:LEU:HD21  | 35:BI:38:LEU:HG    | 1.93                     | 0.51              |
| 37:BO:87:ILE:HG22  | 37:BO:88:ASN:N     | 2.26                     | 0.51              |
| 43:BU:91:ASP:OD2   | 43:BU:96:ALA:CB    | 2.54                     | 0.51              |
| 44:BV:99:ILE:CD1   | 44:BV:99:ILE:N     | 2.74                     | 0.51              |
| 45:BW:99:ARG:HH11  | 45:BW:99:ARG:HG2   | 1.76                     | 0.51              |
| 47:BY:2:ARG:HA     | 47:BY:2:ARG:HH11   | 1.76                     | 0.51              |
| 1:CA:539:A:OP1     | 12:CL:111:LYS:HE2  | 2.11                     | 0.51              |
| 1:CA:544:G:H2'     | 1:CA:545:C:H6      | 1.76                     | 0.51              |
| 1:CA:895:G:H2'     | 1:CA:896:C:C6      | 2.46                     | 0.51              |
| 1:CA:939:G:H5''    | 7:CG:102:ARG:CZ    | 2.40                     | 0.51              |
| 1:CA:1074:G:O4'    | 2:CB:104:ASN:ND2   | 2.44                     | 0.51              |
| 2:CB:82:ARG:HG2    | 2:CB:86:GLU:CD     | 2.31                     | 0.51              |
| 3:CC:103:VAL:O     | 3:CC:103:VAL:HG12  | 2.11                     | 0.51              |
| 3:CC:92:ALA:HA     | 3:CC:95:THR:O      | 2.10                     | 0.51              |
| 4:CD:138:TYR:CD2   | 4:CD:138:TYR:C     | 2.85                     | 0.51              |
| 4:CD:108:LEU:HD11  | 4:CD:174:LEU:HB3   | 1.93                     | 0.51              |
| 4:CD:4:TYR:HD2     | 4:CD:5:ILE:N       | 2.08                     | 0.51              |
| 1:CA:406:G:H5'     | 4:CD:5:ILE:HG21    | 1.93                     | 0.51              |
| 5:CE:110:LEU:HA    | 5:CE:113:ALA:HB3   | 1.93                     | 0.51              |
| 8:CH:97:VAL:HG13   | 8:CH:98:LYS:N      | 2.25                     | 0.51              |
| 10:CJ:30:SER:HB3   | 10:CJ:80:LYS:HE2   | 1.93                     | 0.51              |
| 13:CM:68:GLY:O     | 13:CM:71:ARG:CB    | 2.53                     | 0.51              |
| 16:CP:42:ARG:C     | 16:CP:43:LYS:HD2   | 2.31                     | 0.51              |
| 16:CP:82:GLN:O     | 16:CP:83:GLU:CB    | 2.58                     | 0.51              |
| 17:CQ:83:ASP:OD1   | 17:CQ:84:LEU:HG    | 2.11                     | 0.51              |
| 50:D1:51:VAL:HG22  | 50:D1:52:ARG:H     | 1.76                     | 0.51              |
| 58:D9:11:CYS:SG    | 58:D9:32:HIS:ND1   | 2.84                     | 0.51              |
| 27:DA:1385:G:O6    | 27:DA:1403:C:N4    | 2.43                     | 0.51              |
| 27:DA:1550:C:H2'   | 27:DA:1551:C:C6    | 2.45                     | 0.51              |
| 27:DA:1558:A:O2'   | 27:DA:1559:G:P     | 2.68                     | 0.51              |
| 27:DA:2134:A:H62   | 27:DA:2157:G:H1'   | 1.75                     | 0.51              |
| 27:DA:2790:A:H2'   | 27:DA:2791:C:H5''  | 1.93                     | 0.51              |
| 27:DA:2821:A:H2'   | 27:DA:2822:G:O4'   | 2.11                     | 0.51              |
| 27:DA:227:A:N6     | 27:DA:410:G:H21    | 2.01                     | 0.51              |
| 27:DA:783:A:C2'    | 27:DA:784:A:O5'    | 2.58                     | 0.51              |
| 30:DD:139:GLY:O    | 30:DD:140:THR:C    | 2.49                     | 0.51              |
| 31:DE:182:LEU:HG   | 31:DE:184:VAL:HG23 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DF:16:GLY:O    | 32:DF:17:ARG:CG    | 2.50                     | 0.51              |
| 32:DF:7:TYR:O     | 32:DF:8:GLN:CB     | 2.58                     | 0.51              |
| 33:DG:125:PHE:CD2 | 33:DG:131:TYR:HB2  | 2.46                     | 0.51              |
| 27:DA:1131:G:N7   | 36:DN:75:TYR:CD2   | 2.79                     | 0.51              |
| 37:DO:104:ARG:NH1 | 37:DO:104:ARG:HB3  | 2.26                     | 0.51              |
| 37:DO:112:MET:O   | 37:DO:115:VAL:HB   | 2.10                     | 0.51              |
| 40:DR:26:LYS:NZ   | 40:DR:71:GLN:CB    | 2.74                     | 0.51              |
| 43:DU:83:LEU:CG   | 43:DU:88:ILE:HD11  | 2.33                     | 0.51              |
| 1:AA:1298:C:H4'   | 1:AA:1299:A:C4     | 2.46                     | 0.51              |
| 1:AA:1437:C:N4    | 1:AA:1464:G:H1     | 2.07                     | 0.51              |
| 1:AA:1514:C:H2'   | 1:AA:1515:C:H6     | 1.76                     | 0.51              |
| 1:AA:186:C:H2'    | 1:AA:187:C:H6      | 1.75                     | 0.51              |
| 1:AA:279:A:C5'    | 1:AA:281:G:H5'     | 2.40                     | 0.51              |
| 1:AA:324:G:N2     | 1:AA:327:A:H8      | 2.09                     | 0.51              |
| 1:AA:418:C:H1'    | 1:AA:540:G:O2'     | 2.10                     | 0.51              |
| 1:AA:616:G:H1'    | 1:AA:625:G:N2      | 2.26                     | 0.51              |
| 1:AA:687:A:H1'    | 1:AA:688:G:OP2     | 2.11                     | 0.51              |
| 1:AA:750:G:N3     | 15:AO:23:GLY:HA3   | 2.25                     | 0.51              |
| 1:AA:784:C:N3     | 1:AA:799:G:C2      | 2.79                     | 0.51              |
| 2:AB:41:ILE:HD12  | 2:AB:41:ILE:N      | 2.26                     | 0.51              |
| 2:AB:48:MET:O     | 2:AB:50:GLU:N      | 2.44                     | 0.51              |
| 3:AC:52:LEU:HD23  | 3:AC:52:LEU:H      | 1.76                     | 0.51              |
| 4:AD:173:TRP:O    | 4:AD:174:LEU:HD23  | 2.11                     | 0.51              |
| 8:AH:53:VAL:HB    | 8:AH:56:LYS:HB2    | 1.93                     | 0.51              |
| 15:AO:39:LEU:O    | 15:AO:43:LEU:HG    | 2.11                     | 0.51              |
| 25:AY:68:C:C3'    | 25:AY:69:C:H5''    | 2.40                     | 0.51              |
| 53:B4:44:CYS:SG   | 53:B4:64:LYS:HB2   | 2.51                     | 0.51              |
| 27:BA:1487:G:H1   | 27:BA:1502:C:N4    | 2.09                     | 0.51              |
| 27:BA:1549:C:O2'  | 27:BA:1550:C:H5'   | 2.10                     | 0.51              |
| 27:BA:1657:C:O2'  | 27:BA:1658:C:H5'   | 2.11                     | 0.51              |
| 27:BA:2048:G:C2   | 27:BA:2621:A:C2    | 2.99                     | 0.51              |
| 27:BA:238:C:H1'   | 27:BA:609:A:H1'    | 1.93                     | 0.51              |
| 27:BA:2550:G:C2'  | 27:BA:2551:C:H5'   | 2.41                     | 0.51              |
| 27:BA:968:G:H2'   | 27:BA:969:U:C6     | 2.46                     | 0.51              |
| 27:BA:1799:G:N1   | 30:BD:178:PRO:HD2  | 2.26                     | 0.51              |
| 33:BG:37:VAL:HB   | 33:BG:99:MET:HG3   | 1.93                     | 0.51              |
| 35:BI:73:GLU:CB   | 35:BI:136:VAL:HG23 | 2.40                     | 0.51              |
| 37:BO:24:VAL:HB   | 37:BO:33:ALA:HB2   | 1.93                     | 0.51              |
| 38:BP:105:LEU:O   | 38:BP:106:LEU:HB3  | 2.11                     | 0.51              |
| 27:BA:624:C:H41   | 38:BP:107:LYS:HZ2  | 1.59                     | 0.51              |
| 39:BQ:43:THR:O    | 39:BQ:47:ILE:HG13  | 2.11                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BR:96:ARG:O     | 40:BR:114:VAL:HA  | 2.11                     | 0.51              |
| 43:BU:96:ALA:C     | 43:BU:98:LEU:N    | 2.64                     | 0.51              |
| 47:BY:27:VAL:CA    | 47:BY:28:LYS:NZ   | 2.67                     | 0.51              |
| 48:BZ:96:GLU:O     | 48:BZ:97:MET:HB3  | 2.10                     | 0.51              |
| 1:CA:155:C:O5'     | 1:CA:155:C:H6     | 1.93                     | 0.51              |
| 1:CA:579:G:C6      | 1:CA:580:U:C4     | 2.99                     | 0.51              |
| 1:CA:652:U:C2'     | 1:CA:653:A:H5''   | 2.41                     | 0.51              |
| 2:CB:136:VAL:O     | 2:CB:140:HIS:HB2  | 2.11                     | 0.51              |
| 2:CB:41:ILE:N      | 2:CB:41:ILE:HD12  | 2.26                     | 0.51              |
| 3:CC:14:ILE:HG23   | 3:CC:15:THR:N     | 2.26                     | 0.51              |
| 3:CC:41:GLY:O      | 3:CC:45:LYS:HG3   | 2.11                     | 0.51              |
| 4:CD:150:GLU:N     | 4:CD:150:GLU:CD   | 2.60                     | 0.51              |
| 5:CE:121:LYS:HG3   | 5:CE:122:GLU:N    | 2.26                     | 0.51              |
| 9:CI:15:ALA:HB2    | 9:CI:65:VAL:CG2   | 2.41                     | 0.51              |
| 12:CL:52:VAL:HG22  | 12:CL:66:TYR:CA   | 2.25                     | 0.51              |
| 1:CA:1226:C:C6     | 13:CM:103:THR:O   | 2.64                     | 0.51              |
| 13:CM:24:GLY:C     | 13:CM:25:ILE:HD12 | 2.30                     | 0.51              |
| 14:CN:16:PHE:O     | 14:CN:18:VAL:N    | 2.44                     | 0.51              |
| 20:CT:12:ALA:O     | 20:CT:15:ARG:HB2  | 2.11                     | 0.51              |
| 20:CT:26:ASN:HD22  | 20:CT:27:LYS:H    | 1.59                     | 0.51              |
| 25:CY:20:A:O2'     | 25:CY:21:A:P      | 2.69                     | 0.51              |
| 25:CY:40:C:H2'     | 25:CY:41:G:C8     | 2.40                     | 0.51              |
| 51:D2:9:GLN:OE1    | 51:D2:56:GLN:HG2  | 2.11                     | 0.51              |
| 27:DA:1419:A:H62   | 27:DA:1578:U:H3   | 1.59                     | 0.51              |
| 27:DA:1799:G:O2'   | 27:DA:1800:C:OP2  | 2.28                     | 0.51              |
| 27:DA:1947:C:O2    | 27:DA:1947:C:H2'  | 2.10                     | 0.51              |
| 27:DA:2043:C:H2'   | 27:DA:2043:C:O2   | 2.10                     | 0.51              |
| 27:DA:2248:C:H2'   | 27:DA:2248:C:O2   | 2.10                     | 0.51              |
| 27:DA:272(E):G:H2' | 27:DA:272(F):C:C6 | 2.46                     | 0.51              |
| 27:DA:2866:U:H5''  | 27:DA:2867:G:OP1  | 2.11                     | 0.51              |
| 27:DA:543:C:O3'    | 27:DA:547:A:P     | 2.70                     | 0.51              |
| 27:DA:784:A:OP1    | 27:DA:2588:G:OP1  | 2.29                     | 0.51              |
| 27:DA:77:C:H2'     | 27:DA:78:A:H8     | 1.75                     | 0.51              |
| 27:DA:814:C:H41    | 38:DP:27:HIS:CD2  | 2.29                     | 0.51              |
| 27:DA:849:A:H2'    | 27:DA:850:C:O4'   | 2.11                     | 0.51              |
| 27:DA:992:C:OP1    | 43:DU:47:TYR:OH   | 2.24                     | 0.51              |
| 29:DC:41:VAL:HG23  | 29:DC:178:ALA:CB  | 2.35                     | 0.51              |
| 27:DA:1567:A:H2'   | 30:DD:86:PRO:HG3  | 1.93                     | 0.51              |
| 31:DE:13:ARG:CB    | 31:DE:22:PRO:HA   | 2.41                     | 0.51              |
| 31:DE:51:PHE:CG    | 31:DE:52:LEU:N    | 2.79                     | 0.51              |
| 27:DA:2831:G:OP2   | 31:DE:58:ARG:NH2  | 2.43                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DF:144:LYS:C   | 32:DF:146:ALA:H    | 2.14                     | 0.51              |
| 32:DF:163:VAL:O   | 32:DF:166:ALA:HB3  | 2.11                     | 0.51              |
| 32:DF:167:ALA:HB1 | 32:DF:173:VAL:HG21 | 1.94                     | 0.51              |
| 34:DH:170:ARG:HG2 | 34:DH:171:LEU:N    | 2.26                     | 0.51              |
| 36:DN:3:THR:HG22  | 36:DN:5:VAL:HG12   | 1.93                     | 0.51              |
| 38:DP:9:ASN:O     | 38:DP:10:PRO:C     | 2.48                     | 0.51              |
| 42:DT:96:ARG:HG2  | 42:DT:96:ARG:NH1   | 2.18                     | 0.51              |
| 44:DV:34:GLU:O    | 44:DV:36:PRO:HD3   | 2.10                     | 0.51              |
| 47:DY:28:LYS:NZ   | 47:DY:28:LYS:N     | 2.57                     | 0.51              |
| 47:DY:28:LYS:O    | 47:DY:38:ILE:HB    | 2.11                     | 0.51              |
| 1:AA:1163:C:H2'   | 1:AA:1164:G:H8     | 1.76                     | 0.50              |
| 1:AA:1213:A:H2'   | 1:AA:1215:G:N7     | 2.26                     | 0.50              |
| 1:AA:1428:A:H2'   | 1:AA:1429:C:H6     | 1.76                     | 0.50              |
| 1:AA:169:C:C6     | 1:AA:170:U:H5      | 2.28                     | 0.50              |
| 1:AA:332:G:OP2    | 20:AT:10:LEU:HD13  | 2.12                     | 0.50              |
| 1:AA:471:G:O2'    | 1:AA:472:A:H8      | 1.94                     | 0.50              |
| 5:AE:110:LEU:HD13 | 5:AE:118:ILE:HG21  | 1.93                     | 0.50              |
| 5:AE:15:ARG:CZ    | 5:AE:26:PHE:CE2    | 2.95                     | 0.50              |
| 8:AH:44:PHE:HE2   | 8:AH:109:ILE:HG22  | 1.76                     | 0.50              |
| 8:AH:108:GLY:CA   | 8:AH:138:TRP:HB3   | 2.40                     | 0.50              |
| 11:AK:18:ARG:O    | 11:AK:33:THR:N     | 2.39                     | 0.50              |
| 11:AK:97:ALA:O    | 11:AK:100:ALA:O    | 2.30                     | 0.50              |
| 13:AM:92:HIS:O    | 13:AM:93:ARG:C     | 2.50                     | 0.50              |
| 14:AN:36:PHE:C    | 14:AN:36:PHE:CD1   | 2.84                     | 0.50              |
| 1:AA:667:G:H4'    | 15:AO:51:HIS:CE1   | 2.46                     | 0.50              |
| 15:AO:81:LEU:C    | 15:AO:81:LEU:HD12  | 2.32                     | 0.50              |
| 1:AA:392:G:H4'    | 16:AP:13:HIS:CE1   | 2.47                     | 0.50              |
| 18:AR:62:GLU:O    | 18:AR:63:GLN:C     | 2.50                     | 0.50              |
| 20:AT:75:ASN:HD22 | 20:AT:75:ASN:H     | 1.53                     | 0.50              |
| 49:B0:70:GLN:HG2  | 49:B0:71:ASP:H     | 1.76                     | 0.50              |
| 51:B2:64:LEU:O    | 51:B2:67:LYS:HB2   | 2.11                     | 0.50              |
| 57:B8:61:LEU:N    | 57:B8:61:LEU:CD1   | 2.72                     | 0.50              |
| 57:B8:63:PRO:HG2  | 57:B8:64:TYR:HD1   | 1.76                     | 0.50              |
| 27:BA:1303:G:N3   | 27:BA:1304:C:C6    | 2.79                     | 0.50              |
| 27:BA:1464:C:HO2' | 27:BA:1528:A:H8    | 1.56                     | 0.50              |
| 27:BA:2264:C:C4   | 27:BA:2265:U:C4    | 2.98                     | 0.50              |
| 27:BA:2308:G:O6   | 27:BA:2310:A:H3'   | 2.11                     | 0.50              |
| 27:BA:2328:A:O2'  | 27:BA:2329:G:H5'   | 2.11                     | 0.50              |
| 27:BA:2516:G:H2'  | 27:BA:2517:C:C5'   | 2.40                     | 0.50              |
| 27:BA:2639:A:N6   | 27:BA:2640:G:C2    | 2.79                     | 0.50              |
| 27:BA:2680:C:H4'  | 31:BE:8:LYS:HZ2    | 1.76                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:571:A:C8     | 27:BA:2030:A:N6    | 2.79                     | 0.50              |
| 27:BA:715:G:H2'    | 27:BA:716:A:H8     | 1.76                     | 0.50              |
| 27:BA:924:C:H2'    | 27:BA:925:C:H6     | 1.76                     | 0.50              |
| 28:BB:44:G:H1'     | 28:BB:47:C:N4      | 2.26                     | 0.50              |
| 28:BB:57:A:C8      | 28:BB:57:A:H5'     | 2.46                     | 0.50              |
| 34:BH:103:LEU:HD22 | 34:BH:123:PHE:HE2  | 1.75                     | 0.50              |
| 27:BA:528:A:N7     | 36:BN:114:ARG:NH1  | 2.58                     | 0.50              |
| 36:BN:67:LEU:HA    | 36:BN:87:LEU:HB3   | 1.93                     | 0.50              |
| 42:BT:48:ILE:O     | 42:BT:50:ILE:HD13  | 2.11                     | 0.50              |
| 48:BZ:156:LEU:HD21 | 48:BZ:162:LEU:HD12 | 1.92                     | 0.50              |
| 1:CA:1038:C:H2'    | 1:CA:1039:C:N3     | 2.27                     | 0.50              |
| 1:CA:1188:A:H4'    | 14:CN:58:LYS:HZ2   | 1.76                     | 0.50              |
| 1:CA:984:C:N4      | 1:CA:1221:G:O6     | 2.44                     | 0.50              |
| 1:CA:426:G:H2'     | 1:CA:427:U:C6      | 2.46                     | 0.50              |
| 1:CA:486:U:O2'     | 1:CA:487:A:H8      | 1.93                     | 0.50              |
| 1:CA:538:G:O3'     | 12:CL:111:LYS:NZ   | 2.41                     | 0.50              |
| 1:CA:577:G:N3      | 1:CA:578:C:C5      | 2.79                     | 0.50              |
| 1:CA:741:G:C2      | 1:CA:742:G:C4      | 2.99                     | 0.50              |
| 1:CA:757:U:H2'     | 1:CA:758:G:O4'     | 2.11                     | 0.50              |
| 2:CB:131:PRO:HG2   | 2:CB:134:GLU:CG    | 2.42                     | 0.50              |
| 3:CC:150:LYS:CD    | 3:CC:201:TYR:HD1   | 2.24                     | 0.50              |
| 8:CH:48:TYR:HA     | 8:CH:60:ARG:O      | 2.11                     | 0.50              |
| 10:CJ:37:PRO:HA    | 10:CJ:72:VAL:HG22  | 1.93                     | 0.50              |
| 10:CJ:47:PHE:N     | 10:CJ:47:PHE:CD1   | 2.79                     | 0.50              |
| 12:CL:81:LEU:HB3   | 12:CL:98:VAL:HB    | 1.92                     | 0.50              |
| 15:CO:70:LEU:CD2   | 15:CO:78:TYR:HA    | 2.41                     | 0.50              |
| 20:CT:51:GLU:O     | 20:CT:55:ILE:HG12  | 2.11                     | 0.50              |
| 27:DA:1412:A:H8    | 27:DA:1412:A:O5'   | 1.94                     | 0.50              |
| 27:DA:194:G:C2     | 27:DA:202:U:H1'    | 2.45                     | 0.50              |
| 27:DA:2158:A:HO2'  | 27:DA:2159:G:H8    | 1.57                     | 0.50              |
| 27:DA:2195:C:O2'   | 27:DA:2196:C:H5'   | 2.11                     | 0.50              |
| 27:DA:2298:A:H2'   | 27:DA:2299:G:C8    | 2.44                     | 0.50              |
| 27:DA:2428:G:N2    | 38:DP:60:MET:CE    | 2.74                     | 0.50              |
| 27:DA:691:C:H42    | 27:DA:771:G:H1     | 1.60                     | 0.50              |
| 27:DA:686:G:H21    | 27:DA:788:A:H61    | 1.55                     | 0.50              |
| 27:DA:909:A:H2'    | 27:DA:912:C:H5     | 1.76                     | 0.50              |
| 27:DA:919:G:H4'    | 28:DB:81:G:C4'     | 2.42                     | 0.50              |
| 28:DB:77:U:H4'     | 48:DZ:83:GLU:OE1   | 2.11                     | 0.50              |
| 28:DB:7:G:O2'      | 41:DS:38:GLN:NE2   | 2.44                     | 0.50              |
| 30:DD:142:VAL:HG22 | 30:DD:143:HIS:N    | 2.26                     | 0.50              |
| 30:DD:158:ALA:O    | 30:DD:161:THR:OG1  | 2.26                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DH:105:LEU:HD22 | 34:DH:105:LEU:N    | 2.26                     | 0.50              |
| 35:DI:10:GLU:OE1   | 35:DI:11:ASN:HB2   | 2.11                     | 0.50              |
| 35:DI:115:ALA:HB3  | 35:DI:129:THR:OG1  | 2.11                     | 0.50              |
| 38:DP:102:ARG:HB3  | 38:DP:102:ARG:NH2  | 2.26                     | 0.50              |
| 41:DS:96:GLY:C     | 41:DS:98:VAL:H     | 2.15                     | 0.50              |
| 43:DU:33:ARG:C     | 43:DU:35:ALA:N     | 2.65                     | 0.50              |
| 1:AA:1011:G:O2'    | 1:AA:1012:U:H5'    | 2.11                     | 0.50              |
| 1:AA:1151:A:O2'    | 1:AA:1152:A:C8     | 2.56                     | 0.50              |
| 1:AA:1278:U:C6     | 1:AA:1278:U:H3'    | 2.45                     | 0.50              |
| 1:AA:1403:C:O2'    | 1:AA:1404:C:H5'    | 2.11                     | 0.50              |
| 1:AA:129(A):G:N2   | 1:AA:189(E):U:HO2' | 2.09                     | 0.50              |
| 1:AA:336:C:H1'     | 1:AA:1468:A:H2     | 1.77                     | 0.50              |
| 1:AA:424:G:H2'     | 1:AA:425:G:C8      | 2.46                     | 0.50              |
| 1:AA:575:G:H4'     | 1:AA:576:G:C5'     | 2.41                     | 0.50              |
| 1:AA:610:G:H2'     | 1:AA:611:A:H8      | 1.75                     | 0.50              |
| 1:AA:736:C:H5''    | 18:AR:72:ARG:HE    | 1.76                     | 0.50              |
| 1:AA:836:G:C6      | 1:AA:851:G:C6      | 3.00                     | 0.50              |
| 1:AA:562:C:H41     | 1:AA:884:U:H2'     | 1.76                     | 0.50              |
| 3:AC:73:PRO:HG3    | 3:AC:105:GLU:HG3   | 1.92                     | 0.50              |
| 7:AG:15:ASP:HB3    | 7:AG:19:GLY:N      | 2.26                     | 0.50              |
| 1:AA:963:G:H21     | 10:AJ:55:LYS:CE    | 2.24                     | 0.50              |
| 10:AJ:6:ILE:CG1    | 10:AJ:72:VAL:O     | 2.57                     | 0.50              |
| 10:AJ:30:SER:OG    | 10:AJ:81:THR:CG2   | 2.58                     | 0.50              |
| 15:AO:66:LEU:C     | 15:AO:68:ARG:H     | 2.14                     | 0.50              |
| 16:AP:74:LEU:HA    | 16:AP:77:ALA:HB3   | 1.93                     | 0.50              |
| 1:AA:128:G:H5'     | 17:AQ:2:PRO:HA     | 1.93                     | 0.50              |
| 17:AQ:74:LEU:O     | 17:AQ:75:ARG:HB3   | 2.12                     | 0.50              |
| 18:AR:19:LYS:O     | 18:AR:20:ALA:HB2   | 2.11                     | 0.50              |
| 18:AR:71:LYS:O     | 18:AR:73:ALA:N     | 2.45                     | 0.50              |
| 1:AA:1326:C:OP1    | 21:AU:12:LYS:HD2   | 2.11                     | 0.50              |
| 24:AX:6:G:N2       | 24:AX:68:C:C2      | 2.79                     | 0.50              |
| 51:B2:4:SER:HA     | 51:B2:7:ARG:HH11   | 1.77                     | 0.50              |
| 27:BA:1175:U:H5''  | 27:BA:1176:G:H8    | 1.75                     | 0.50              |
| 27:BA:1281:G:H2'   | 27:BA:1281:G:N3    | 2.27                     | 0.50              |
| 27:BA:1593:G:H3'   | 27:BA:1594:G:H8    | 1.76                     | 0.50              |
| 27:BA:1810:A:H2'   | 27:BA:1811:G:H5'   | 1.93                     | 0.50              |
| 27:BA:2302:G:C2'   | 27:BA:2303:G:H5'   | 2.41                     | 0.50              |
| 27:BA:2313:C:C5    | 27:BA:2314:C:H5    | 2.29                     | 0.50              |
| 27:BA:251:A:H5''   | 38:BP:51:PHE:CZ    | 2.46                     | 0.50              |
| 27:BA:303:U:O2'    | 27:BA:304:G:H5'    | 2.11                     | 0.50              |
| 27:BA:39:C:H2'     | 27:BA:40:C:C6      | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:624:C:O2'   | 27:BA:625:G:H5'   | 2.11                     | 0.50              |
| 28:BB:17:C:H2'    | 28:BB:18:G:O4'    | 2.11                     | 0.50              |
| 34:BH:83:TYR:HA   | 34:BH:135:GLY:H   | 1.76                     | 0.50              |
| 34:BH:38:SER:OG   | 34:BH:40:GLU:HG3  | 2.11                     | 0.50              |
| 35:BI:129:THR:HA  | 35:BI:137:PRO:HA  | 1.92                     | 0.50              |
| 42:BT:28:VAL:HG11 | 42:BT:46:GLU:HB2  | 1.94                     | 0.50              |
| 42:BT:57:PHE:CG   | 42:BT:58:ASN:N    | 2.80                     | 0.50              |
| 42:BT:65:LYS:HZ1  | 42:BT:66:VAL:HG23 | 1.74                     | 0.50              |
| 42:BT:78:LEU:C    | 42:BT:79:HIS:ND1  | 2.65                     | 0.50              |
| 46:BX:82:GLN:HG3  | 46:BX:83:VAL:N    | 2.26                     | 0.50              |
| 1:CA:1301:U:OP2   | 1:CA:1303:C:N4    | 2.44                     | 0.50              |
| 1:CA:1408:A:O2'   | 1:CA:1409:C:H5'   | 2.10                     | 0.50              |
| 1:CA:263:A:H2'    | 1:CA:264:U:C6     | 2.46                     | 0.50              |
| 1:CA:293:G:H1     | 1:CA:304:U:H3     | 1.59                     | 0.50              |
| 1:CA:37:U:H2'     | 1:CA:38:G:O4'     | 2.10                     | 0.50              |
| 1:CA:708:C:O2'    | 1:CA:709:G:H5'    | 2.11                     | 0.50              |
| 1:CA:913:A:O2'    | 1:CA:914:A:OP2    | 2.30                     | 0.50              |
| 1:CA:885:G:H1'    | 1:CA:914:A:N1     | 2.26                     | 0.50              |
| 2:CB:224:GLN:CG   | 2:CB:229:VAL:HG22 | 2.41                     | 0.50              |
| 3:CC:189:ALA:O    | 3:CC:195:VAL:HG12 | 2.11                     | 0.50              |
| 7:CG:26:PHE:CG    | 7:CG:62:PHE:HE1   | 2.30                     | 0.50              |
| 7:CG:72:ARG:C     | 7:CG:73:MET:HG3   | 2.31                     | 0.50              |
| 8:CH:82:HIS:O     | 8:CH:83:ILE:HB    | 2.11                     | 0.50              |
| 13:CM:14:ARG:N    | 13:CM:44:ARG:NH1  | 2.56                     | 0.50              |
| 20:CT:48:LYS:HB3  | 20:CT:51:GLU:CG   | 2.42                     | 0.50              |
| 27:DA:1055:G:H2'  | 27:DA:1108:U:C6   | 2.46                     | 0.50              |
| 27:DA:1348:G:C2'  | 27:DA:1349:A:H5'' | 2.41                     | 0.50              |
| 27:DA:1455:G:H2'  | 27:DA:1456:G:H8   | 1.76                     | 0.50              |
| 27:DA:1700:A:H2'  | 27:DA:1701:A:O4'  | 2.11                     | 0.50              |
| 27:DA:1823:G:O2'  | 27:DA:1824:G:H5'  | 2.11                     | 0.50              |
| 27:DA:1794:U:O4'  | 27:DA:1900:A:C2   | 2.64                     | 0.50              |
| 27:DA:2140:C:H1'  | 27:DA:2152:G:N2   | 2.26                     | 0.50              |
| 27:DA:356:G:H2'   | 27:DA:356:G:N3    | 2.26                     | 0.50              |
| 27:DA:45:C:H2'    | 27:DA:47:C:H6     | 1.76                     | 0.50              |
| 27:DA:507:A:H4'   | 27:DA:509:C:C5    | 2.46                     | 0.50              |
| 28:DB:35:U:O2'    | 28:DB:36:C:O5'    | 2.17                     | 0.50              |
| 28:DB:45:A:C1'    | 33:DG:95:ARG:NH1  | 2.74                     | 0.50              |
| 29:DC:20:TYR:CG   | 29:DC:21:THR:N    | 2.78                     | 0.50              |
| 31:DE:29:GLY:CA   | 31:DE:180:ASN:HB3 | 2.41                     | 0.50              |
| 31:DE:92:THR:O    | 31:DE:95:ILE:HB   | 2.11                     | 0.50              |
| 33:DG:105:LYS:HE2 | 33:DG:143:GLU:OE2 | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DH:65:HIS:ND1   | 34:DH:65:HIS:O     | 2.44                     | 0.50              |
| 34:DH:98:LEU:HG    | 34:DH:98:LEU:O     | 2.12                     | 0.50              |
| 36:DN:112:LEU:O    | 36:DN:115:ARG:HB3  | 2.11                     | 0.50              |
| 38:DP:83:VAL:O     | 38:DP:115:LEU:HD23 | 2.12                     | 0.50              |
| 38:DP:135:LEU:HD13 | 38:DP:135:LEU:C    | 2.32                     | 0.50              |
| 40:DR:56:LYS:HD2   | 40:DR:88:ARG:HA    | 1.93                     | 0.50              |
| 42:DT:129:ARG:NH1  | 42:DT:131:ALA:O    | 2.44                     | 0.50              |
| 46:DX:28:PHE:O     | 46:DX:30:VAL:HG13  | 2.11                     | 0.50              |
| 47:DY:96:ILE:HG22  | 47:DY:97:ARG:H     | 1.76                     | 0.50              |
| 1:AA:1357:A:N7     | 1:AA:1358:U:C4     | 2.79                     | 0.50              |
| 1:AA:139:G:H2'     | 1:AA:140:A:H8      | 1.77                     | 0.50              |
| 1:AA:274:A:O2'     | 1:AA:275:G:H8      | 1.94                     | 0.50              |
| 1:AA:450:G:H4'     | 16:AP:41:PRO:O     | 2.10                     | 0.50              |
| 1:AA:486:U:H5'     | 1:AA:486:U:C6      | 2.42                     | 0.50              |
| 1:AA:577:G:N3      | 1:AA:578:C:C5      | 2.79                     | 0.50              |
| 1:AA:605:U:O2'     | 1:AA:606:G:H5'     | 2.11                     | 0.50              |
| 1:AA:862:C:O2'     | 1:AA:863:U:H5'     | 2.10                     | 0.50              |
| 2:AB:14:GLY:C      | 2:AB:15:VAL:HG22   | 2.31                     | 0.50              |
| 2:AB:28:PHE:CD2    | 2:AB:194:PRO:HD3   | 2.46                     | 0.50              |
| 3:AC:125:GLU:HG2   | 3:AC:190:ARG:O     | 2.10                     | 0.50              |
| 3:AC:73:PRO:C      | 3:AC:75:VAL:N      | 2.65                     | 0.50              |
| 4:AD:59:ARG:NH2    | 4:AD:66:ARG:NH2    | 2.59                     | 0.50              |
| 11:AK:23:ALA:HB1   | 11:AK:88:GLY:HA3   | 1.92                     | 0.50              |
| 16:AP:1:MET:HG2    | 16:AP:2:VAL:N      | 2.26                     | 0.50              |
| 1:AA:472:A:H5''    | 16:AP:80:PHE:HB3   | 1.93                     | 0.50              |
| 20:AT:63:ILE:O     | 20:AT:65:LYS:N     | 2.44                     | 0.50              |
| 23:AW:42:G:H3'     | 23:AW:43:C:H5''    | 1.92                     | 0.50              |
| 24:AX:51:C:H2'     | 24:AX:52:G:C8      | 2.46                     | 0.50              |
| 45:BW:35:ILE:HG23  | 54:B5:28:PRO:HD2   | 1.93                     | 0.50              |
| 27:BA:1006:C:H1'   | 36:BN:106:MET:CG   | 2.37                     | 0.50              |
| 27:BA:70:G:O2'     | 27:BA:114:U:C5     | 2.60                     | 0.50              |
| 27:BA:1293:C:H2'   | 27:BA:1294:U:C6    | 2.46                     | 0.50              |
| 27:BA:1331:A:HO2'  | 27:BA:1332:G:H8    | 1.58                     | 0.50              |
| 27:BA:1480:G:C5    | 27:BA:1481:U:C5    | 3.00                     | 0.50              |
| 27:BA:1803:A:O2'   | 30:BD:259:THR:HG21 | 2.10                     | 0.50              |
| 1:AA:784:C:H4'     | 27:BA:1837:C:OP1   | 2.11                     | 0.50              |
| 27:BA:1957:C:H2'   | 27:BA:1958:C:H6    | 1.76                     | 0.50              |
| 27:BA:2175:C:H1'   | 29:BC:215:THR:N    | 2.26                     | 0.50              |
| 27:BA:2228:G:OP1   | 30:BD:261:LYS:CE   | 2.60                     | 0.50              |
| 27:BA:2287:A:C5    | 27:BA:2289:G:C5    | 3.00                     | 0.50              |
| 27:BA:2492:U:H2'   | 27:BA:2493:U:C6    | 2.46                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:25:U:C2'     | 27:BA:26:G:O5'     | 2.59                     | 0.50              |
| 27:BA:271(M):G:O2' | 27:BA:271(N):U:H3' | 2.11                     | 0.50              |
| 27:BA:399:G:C2     | 27:BA:400:G:H1'    | 2.46                     | 0.50              |
| 27:BA:689:A:O2'    | 27:BA:690:G:H5'    | 2.10                     | 0.50              |
| 30:BD:158:ALA:HB3  | 30:BD:161:THR:HG23 | 1.92                     | 0.50              |
| 30:BD:230:ASP:O    | 30:BD:231:HIS:HB2  | 2.11                     | 0.50              |
| 31:BE:9:VAL:HG11   | 31:BE:25:VAL:CG1   | 2.40                     | 0.50              |
| 32:BF:21:ALA:C     | 32:BF:23:ASP:N     | 2.64                     | 0.50              |
| 33:BG:172:LEU:O    | 33:BG:175:LEU:N    | 2.43                     | 0.50              |
| 35:BI:29:TYR:O     | 35:BI:33:ARG:HB2   | 2.11                     | 0.50              |
| 37:BO:51:ALA:O     | 37:BO:52:VAL:HB    | 2.11                     | 0.50              |
| 38:BP:7:ARG:O      | 38:BP:10:PRO:HD3   | 2.11                     | 0.50              |
| 43:BU:48:ALA:O     | 43:BU:51:LYS:HB2   | 2.12                     | 0.50              |
| 44:BV:45:THR:O     | 44:BV:46:VAL:HG12  | 2.12                     | 0.50              |
| 47:BY:17:SER:O     | 47:BY:21:LYS:HB2   | 2.12                     | 0.50              |
| 47:BY:24:VAL:HG12  | 47:BY:25:GLY:N     | 2.25                     | 0.50              |
| 1:CA:1001(A):G:C8  | 1:CA:1002:G:C8     | 2.99                     | 0.50              |
| 1:CA:1036:G:H5''   | 1:CA:1037:C:C5     | 2.46                     | 0.50              |
| 1:CA:1139:G:H5'    | 1:CA:1140:C:OP1    | 2.12                     | 0.50              |
| 1:CA:1181:G:H2'    | 1:CA:1182:G:C5     | 2.43                     | 0.50              |
| 1:CA:1212:U:OP1    | 1:CA:1212:U:H4'    | 2.11                     | 0.50              |
| 1:CA:1385:G:C2'    | 1:CA:1386:G:H5'    | 2.41                     | 0.50              |
| 1:CA:274:A:HO2'    | 1:CA:275:G:C5'     | 2.23                     | 0.50              |
| 1:CA:383:A:H2'     | 1:CA:384:G:H5'     | 1.94                     | 0.50              |
| 1:CA:762:C:H2'     | 1:CA:763:G:H8      | 1.75                     | 0.50              |
| 1:CA:848:C:O2'     | 1:CA:849:C:H5'     | 2.10                     | 0.50              |
| 1:CA:973:G:C5      | 1:CA:974:A:N7      | 2.79                     | 0.50              |
| 3:CC:140:ARG:O     | 3:CC:143:GLU:N     | 2.45                     | 0.50              |
| 3:CC:162:GLN:HA    | 3:CC:162:GLN:OE1   | 2.10                     | 0.50              |
| 4:CD:8:VAL:CG1     | 4:CD:21:LEU:HD13   | 2.36                     | 0.50              |
| 4:CD:3:ARG:HG2     | 4:CD:118:ARG:NE    | 2.27                     | 0.50              |
| 5:CE:101:ILE:HG12  | 5:CE:119:LEU:HA    | 1.92                     | 0.50              |
| 5:CE:126:ARG:NH1   | 5:CE:126:ARG:HG3   | 2.25                     | 0.50              |
| 8:CH:21:LYS:O      | 8:CH:65:TYR:OH     | 2.28                     | 0.50              |
| 1:CA:653:A:H1'     | 8:CH:56:LYS:NZ     | 2.26                     | 0.50              |
| 12:CL:31:ARG:O     | 12:CL:58:THR:HG23  | 2.12                     | 0.50              |
| 12:CL:23:ALA:HA    | 12:CL:95:TYR:HE2   | 1.76                     | 0.50              |
| 15:CO:53:HIS:O     | 15:CO:56:LEU:N     | 2.44                     | 0.50              |
| 12:CL:5:ASN:HB2    | 17:CQ:34:LYS:NZ    | 2.26                     | 0.50              |
| 27:DA:111:A:H4'    | 51:D2:69:ARG:HH21  | 1.76                     | 0.50              |
| 27:DA:1150:C:O2'   | 27:DA:1151:G:H5'   | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1818:U:C6    | 30:DD:157:ARG:NH1  | 2.79                     | 0.50              |
| 27:DA:1818:U:H2'   | 30:DD:157:ARG:HG3  | 1.92                     | 0.50              |
| 27:DA:2261:C:OP1   | 49:D0:17:GLN:CD    | 2.50                     | 0.50              |
| 27:DA:2295:C:C2    | 27:DA:2296:U:H5    | 2.29                     | 0.50              |
| 27:DA:2315:G:H2'   | 27:DA:2316:C:C6    | 2.46                     | 0.50              |
| 27:DA:2425:A:H5''  | 27:DA:2427:C:H5'   | 1.91                     | 0.50              |
| 27:DA:2500:U:H2'   | 27:DA:2504:U:H5    | 1.76                     | 0.50              |
| 27:DA:329:G:O2'    | 27:DA:330:A:OP1    | 2.25                     | 0.50              |
| 27:DA:944:G:H5''   | 27:DA:945:A:H5'    | 1.93                     | 0.50              |
| 29:DC:187:ASP:C    | 29:DC:189:ILE:H    | 2.15                     | 0.50              |
| 29:DC:36:LYS:HA    | 29:DC:36:LYS:HZ2   | 1.77                     | 0.50              |
| 29:DC:66:HIS:HB2   | 29:DC:189:ILE:CB   | 2.42                     | 0.50              |
| 30:DD:124:PRO:HG2  | 30:DD:129:ASN:ND2  | 2.26                     | 0.50              |
| 30:DD:253:GLN:HB2  | 30:DD:257:LEU:HD12 | 1.93                     | 0.50              |
| 30:DD:43:ARG:HH11  | 30:DD:44:ASN:CG    | 2.14                     | 0.50              |
| 31:DE:111:ARG:HD2  | 31:DE:160:TYR:HE1  | 1.71                     | 0.50              |
| 31:DE:119:ARG:CG   | 31:DE:160:TYR:HB2  | 2.40                     | 0.50              |
| 32:DF:170:LEU:HD21 | 32:DF:172:TRP:CZ2  | 2.47                     | 0.50              |
| 34:DH:147:ASN:ND2  | 34:DH:147:ASN:H    | 2.08                     | 0.50              |
| 35:DI:72:LEU:CD2   | 35:DI:75:LEU:HD23  | 2.41                     | 0.50              |
| 36:DN:47:ALA:O     | 36:DN:119:ARG:NH2  | 2.44                     | 0.50              |
| 40:DR:14:SER:C     | 40:DR:16:HIS:N     | 2.64                     | 0.50              |
| 40:DR:63:ARG:NH1   | 40:DR:80:PHE:CG    | 2.79                     | 0.50              |
| 41:DS:59:LYS:NZ    | 41:DS:68:GLN:NE2   | 2.58                     | 0.50              |
| 41:DS:82:ILE:CG2   | 41:DS:83:LYS:N     | 2.74                     | 0.50              |
| 43:DU:65:ILE:HG12  | 43:DU:96:ALA:HB1   | 1.93                     | 0.50              |
| 47:DY:95:LYS:HD3   | 47:DY:99:CYS:O     | 2.11                     | 0.50              |
| 48:DZ:44:ASP:O     | 48:DZ:45:LYS:C     | 2.49                     | 0.50              |
| 1:AA:1008:C:H2'    | 1:AA:1009:G:O4'    | 2.10                     | 0.50              |
| 1:AA:1350:A:O5'    | 1:AA:1350:A:H8     | 1.94                     | 0.50              |
| 1:AA:1358:U:OP1    | 14:AN:35:ARG:HG3   | 2.12                     | 0.50              |
| 1:AA:221:C:C2'     | 1:AA:222:U:H5'     | 2.41                     | 0.50              |
| 1:AA:234:C:O2'     | 1:AA:235:C:H5'     | 2.11                     | 0.50              |
| 1:AA:339:C:H2'     | 1:AA:340:U:H6      | 1.76                     | 0.50              |
| 1:AA:797:C:O2'     | 1:AA:798:G:H5'     | 2.11                     | 0.50              |
| 3:AC:155:GLY:CA    | 3:AC:163:ALA:HB1   | 2.28                     | 0.50              |
| 3:AC:184:TYR:CG    | 3:AC:185:GLY:N     | 2.79                     | 0.50              |
| 3:AC:28:GLN:HA     | 3:AC:31:HIS:NE2    | 2.26                     | 0.50              |
| 5:AE:7:GLU:O       | 5:AE:8:GLU:HB3     | 2.11                     | 0.50              |
| 6:AF:88:VAL:HG12   | 6:AF:89:MET:N      | 2.26                     | 0.50              |
| 2:AB:181:PHE:HE1   | 8:AH:70:GLN:HB2    | 1.76                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:AI:71:SER:O      | 9:AI:74:ILE:HB    | 2.10                     | 0.50              |
| 11:AK:79:SER:HB2   | 11:AK:106:LYS:CE  | 2.40                     | 0.50              |
| 12:AL:31:ARG:HG3   | 12:AL:102:TYR:HE1 | 1.75                     | 0.50              |
| 13:AM:96:LEU:HD23  | 13:AM:97:PRO:HD2  | 1.92                     | 0.50              |
| 18:AR:55:ARG:HG3   | 18:AR:55:ARG:NH1  | 2.24                     | 0.50              |
| 19:AS:19:VAL:HG13  | 19:AS:47:HIS:NE2  | 2.26                     | 0.50              |
| 20:AT:77:ALA:O     | 20:AT:81:LYS:HG3  | 2.11                     | 0.50              |
| 25:AY:10:G:H8      | 25:AY:10:G:OP1    | 1.94                     | 0.50              |
| 27:BA:459:U:OP2    | 56:B7:39:ARG:NH1  | 2.44                     | 0.50              |
| 27:BA:1045:A:H4'   | 27:BA:1047:G:O4'  | 2.11                     | 0.50              |
| 27:BA:1333:C:H2'   | 27:BA:1334:G:H8   | 1.76                     | 0.50              |
| 27:BA:1849:G:H2'   | 27:BA:1850:G:H8   | 1.75                     | 0.50              |
| 27:BA:2160:G:H2'   | 27:BA:2161:C:C6   | 2.47                     | 0.50              |
| 27:BA:397:G:H2'    | 27:BA:398:G:H8    | 1.76                     | 0.50              |
| 27:BA:482:A:H1'    | 27:BA:498:G:N2    | 2.26                     | 0.50              |
| 27:BA:523:C:H4'    | 27:BA:540:C:O2    | 2.12                     | 0.50              |
| 27:BA:686:G:H21    | 27:BA:788:A:H61   | 1.58                     | 0.50              |
| 31:BE:11:MET:HB2   | 31:BE:23:VAL:O    | 2.12                     | 0.50              |
| 32:BF:160:ASN:C    | 32:BF:162:LEU:N   | 2.65                     | 0.50              |
| 32:BF:160:ASN:HD22 | 32:BF:162:LEU:H   | 1.60                     | 0.50              |
| 32:BF:70:THR:C     | 32:BF:72:ARG:N    | 2.64                     | 0.50              |
| 34:BH:32:GLU:HG2   | 34:BH:33:LEU:N    | 2.27                     | 0.50              |
| 34:BH:53:GLU:O     | 34:BH:54:ARG:CB   | 2.60                     | 0.50              |
| 36:BN:94:HIS:N     | 36:BN:95:PRO:CD   | 2.75                     | 0.50              |
| 38:BP:140:ALA:O    | 38:BP:141:ALA:HB3 | 2.11                     | 0.50              |
| 38:BP:35:HIS:O     | 38:BP:36:LYS:CB   | 2.59                     | 0.50              |
| 39:BQ:137:TYR:O    | 39:BQ:138:ASP:C   | 2.48                     | 0.50              |
| 27:BA:1651:G:OP2   | 40:BR:40:LYS:HE2  | 2.11                     | 0.50              |
| 41:BS:16:ASN:O     | 41:BS:19:LYS:HB3  | 2.10                     | 0.50              |
| 41:BS:95:HIS:O     | 41:BS:97:ARG:HG3  | 2.12                     | 0.50              |
| 42:BT:91:ARG:HA    | 42:BT:116:ALA:HA  | 1.92                     | 0.50              |
| 43:BU:24:TYR:CD1   | 43:BU:38:THR:HG21 | 2.46                     | 0.50              |
| 36:BN:4:TYR:HB2    | 43:BU:64:ARG:NH2  | 2.26                     | 0.50              |
| 44:BV:19:LYS:HG3   | 44:BV:20:LEU:N    | 2.27                     | 0.50              |
| 47:BY:51:VAL:O     | 47:BY:52:SER:CB   | 2.60                     | 0.50              |
| 1:CA:101:A:C2'     | 1:CA:102:G:H5'    | 2.42                     | 0.50              |
| 1:CA:1096:C:H2'    | 1:CA:1097:C:C6    | 2.46                     | 0.50              |
| 1:CA:1202:G:O2'    | 1:CA:1203:C:H5'   | 2.11                     | 0.50              |
| 1:CA:986:A:N1      | 1:CA:1220:G:C2    | 2.80                     | 0.50              |
| 1:CA:1521:G:C5     | 1:CA:1522:U:C5    | 2.99                     | 0.50              |
| 1:CA:273:A:H1'     | 17:CQ:16:GLN:OE1  | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:769:G:HO2'    | 1:CA:770:C:H5'     | 1.76                     | 0.50              |
| 5:CE:11:ILE:HG22   | 5:CE:12:LEU:N      | 2.19                     | 0.50              |
| 7:CG:100:ALA:O     | 7:CG:101:LEU:C     | 2.50                     | 0.50              |
| 1:CA:1346:A:C5     | 7:CG:10:ARG:CZ     | 2.94                     | 0.50              |
| 7:CG:49:ILE:O      | 7:CG:53:LYS:HB2    | 2.12                     | 0.50              |
| 8:CH:11:THR:O      | 8:CH:15:ASN:ND2    | 2.45                     | 0.50              |
| 11:CK:59:TYR:OH    | 11:CK:63:LEU:HD21  | 2.12                     | 0.50              |
| 13:CM:20:THR:O     | 13:CM:22:ILE:N     | 2.42                     | 0.50              |
| 13:CM:4:ILE:CG2    | 13:CM:5:ALA:H      | 2.10                     | 0.50              |
| 15:CO:12:ILE:C     | 15:CO:14:GLU:N     | 2.62                     | 0.50              |
| 49:D0:53:MET:HE3   | 49:D0:57:PHE:HD1   | 1.76                     | 0.50              |
| 51:D2:14:ARG:HG3   | 51:D2:14:ARG:HH11  | 1.77                     | 0.50              |
| 57:D8:63:PRO:O     | 57:D8:64:TYR:O     | 2.29                     | 0.50              |
| 27:DA:1824:G:O2'   | 27:DA:1825:A:H5'   | 2.12                     | 0.50              |
| 27:DA:204:A:H1'    | 27:DA:206:U:C6     | 2.46                     | 0.50              |
| 27:DA:2645:G:H3'   | 27:DA:2646:C:H5'   | 1.92                     | 0.50              |
| 27:DA:2683:C:P     | 42:DT:53:ARG:NH2   | 2.77                     | 0.50              |
| 27:DA:2853:C:H2'   | 27:DA:2854:G:C8    | 2.46                     | 0.50              |
| 27:DA:416:C:H2'    | 27:DA:416:C:O2     | 2.11                     | 0.50              |
| 27:DA:614(C):A:O2' | 27:DA:615:G:C8     | 2.64                     | 0.50              |
| 27:DA:743:G:C2'    | 27:DA:744:G:H5'    | 2.42                     | 0.50              |
| 27:DA:747:U:O2     | 27:DA:2014:A:H1'   | 2.12                     | 0.50              |
| 27:DA:925:C:H2'    | 27:DA:926:A:O4'    | 2.12                     | 0.50              |
| 29:DC:83:ILE:HD11  | 29:DC:95:GLY:O     | 2.12                     | 0.50              |
| 32:DF:177:ALA:HB1  | 32:DF:178:PRO:CD   | 2.40                     | 0.50              |
| 34:DH:86:GLU:HB3   | 34:DH:132:ARG:HD3  | 1.93                     | 0.50              |
| 36:DN:89:LYS:NZ    | 36:DN:89:LYS:CB    | 2.74                     | 0.50              |
| 37:DO:106:LEU:HB3  | 37:DO:111:PHE:HB2  | 1.93                     | 0.50              |
| 38:DP:58:THR:C     | 38:DP:60:MET:N     | 2.64                     | 0.50              |
| 38:DP:95:VAL:CG2   | 38:DP:100:LEU:HD21 | 2.42                     | 0.50              |
| 39:DQ:18:LYS:HB2   | 39:DQ:98:LYS:NZ    | 2.27                     | 0.50              |
| 27:DA:870:A:OP1    | 39:DQ:6:ARG:NE     | 2.44                     | 0.50              |
| 41:DS:49:VAL:HG12  | 41:DS:50:SER:N     | 2.26                     | 0.50              |
| 44:DV:68:LYS:HA    | 44:DV:68:LYS:HZ2   | 1.77                     | 0.50              |
| 46:DX:60:ARG:NH2   | 56:D7:47:ARG:NE    | 2.59                     | 0.50              |
| 1:AA:1316:G:H1'    | 1:AA:1360:A:C2     | 2.47                     | 0.50              |
| 1:AA:346:G:O2'     | 1:AA:347:G:O4'     | 2.30                     | 0.50              |
| 2:AB:91:PRO:HG2    | 2:AB:155:LEU:HB2   | 1.92                     | 0.50              |
| 2:AB:95:GLN:HG3    | 2:AB:148:TYR:HD1   | 1.77                     | 0.50              |
| 3:AC:11:ARG:O      | 3:AC:15:THR:N      | 2.44                     | 0.50              |
| 3:AC:70:VAL:CG1    | 3:AC:71:ALA:N      | 2.74                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:92:VAL:O      | 4:AD:93:PHE:C      | 2.50                     | 0.50              |
| 6:AF:99:ALA:HB2    | 18:AR:31:LEU:HD13  | 1.93                     | 0.50              |
| 1:AA:875:C:H1'     | 8:AH:15:ASN:OD1    | 2.12                     | 0.50              |
| 12:AL:49:LEU:N     | 12:AL:49:LEU:HD22  | 2.27                     | 0.50              |
| 13:AM:38:GLY:C     | 13:AM:39:ILE:HG13  | 2.32                     | 0.50              |
| 19:AS:29:ARG:HD2   | 19:AS:29:ARG:C     | 2.32                     | 0.50              |
| 50:B1:5:CYS:HA     | 50:B1:61:ARG:O     | 2.10                     | 0.50              |
| 52:B3:8:LEU:HA     | 52:B3:54:VAL:HG22  | 1.94                     | 0.50              |
| 57:B8:17:THR:O     | 57:B8:19:SER:N     | 2.41                     | 0.50              |
| 27:BA:1718:G:C8    | 27:BA:1718:G:H5'   | 2.42                     | 0.50              |
| 27:BA:1681:G:H1'   | 27:BA:1763:G:H5'   | 1.94                     | 0.50              |
| 27:BA:1986:A:C2'   | 27:BA:1987:G:H5'   | 2.42                     | 0.50              |
| 27:BA:2287:A:O2'   | 27:BA:2288:A:H5''  | 2.11                     | 0.50              |
| 27:BA:2555:U:O2'   | 27:BA:2556:C:H5'   | 2.11                     | 0.50              |
| 27:BA:2586:C:H5'   | 27:BA:2586:C:C6    | 2.47                     | 0.50              |
| 27:BA:423:A:H8     | 27:BA:423:A:O5'    | 1.95                     | 0.50              |
| 27:BA:778:G:C6     | 27:BA:779:U:N3     | 2.78                     | 0.50              |
| 27:BA:61:G:H1      | 27:BA:94:C:H42     | 1.58                     | 0.50              |
| 29:BC:19:VAL:HG12  | 29:BC:20:TYR:CD1   | 2.45                     | 0.50              |
| 30:BD:97:TYR:HB2   | 30:BD:101:GLU:O    | 2.11                     | 0.50              |
| 30:BD:204:ILE:HG13 | 30:BD:204:ILE:O    | 2.12                     | 0.50              |
| 33:BG:24:GLY:O     | 33:BG:26:GLN:NE2   | 2.45                     | 0.50              |
| 33:BG:4:ASP:O      | 33:BG:4:ASP:OD1    | 2.29                     | 0.50              |
| 35:BI:5:LEU:CD2    | 35:BI:13:GLY:HA2   | 2.33                     | 0.50              |
| 38:BP:104:GLY:N    | 38:BP:105:LEU:HD23 | 2.27                     | 0.50              |
| 38:BP:138:LEU:O    | 38:BP:140:ALA:N    | 2.43                     | 0.50              |
| 39:BQ:19:GLY:O     | 39:BQ:20:ALA:CB    | 2.59                     | 0.50              |
| 44:BV:22:VAL:O     | 44:BV:23:GLU:CB    | 2.57                     | 0.50              |
| 27:BA:1339:G:OP1   | 46:BX:14:SER:HB2   | 2.10                     | 0.50              |
| 1:CA:1004:A:C5'    | 1:CA:1025:U:H3     | 2.24                     | 0.50              |
| 1:CA:1098:C:H2'    | 1:CA:1099:G:O4'    | 2.12                     | 0.50              |
| 1:CA:1125:U:H2'    | 1:CA:1126:U:OP2    | 2.12                     | 0.50              |
| 1:CA:1244:C:H2'    | 1:CA:1245:A:C8     | 2.46                     | 0.50              |
| 1:CA:1505:G:H4'    | 1:CA:1506:U:C5'    | 2.41                     | 0.50              |
| 1:CA:192:U:H1'     | 20:CT:103:GLY:O    | 2.12                     | 0.50              |
| 1:CA:357:G:O2'     | 1:CA:358:U:H5'     | 2.11                     | 0.50              |
| 1:CA:37:U:H2'      | 1:CA:38:G:C8       | 2.47                     | 0.50              |
| 1:CA:599:C:H5''    | 8:CH:96:GLY:CA     | 2.41                     | 0.50              |
| 1:CA:930:C:O2'     | 1:CA:931:C:H5'     | 2.11                     | 0.50              |
| 3:CC:3:ASN:N       | 3:CC:3:ASN:OD1     | 2.44                     | 0.50              |
| 4:CD:25:ARG:C      | 4:CD:27:TYR:N      | 2.65                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:CH:102:ARG:N     | 8:CH:102:ARG:HE   | 2.09                     | 0.50              |
| 8:CH:95:VAL:HG23   | 8:CH:95:VAL:O     | 2.12                     | 0.50              |
| 9:CI:27:THR:HG22   | 9:CI:31:GLN:H     | 1.75                     | 0.50              |
| 9:CI:92:TYR:O      | 9:CI:95:LYS:HG3   | 2.12                     | 0.50              |
| 10:CJ:44:VAL:CG1   | 10:CJ:46:ARG:HG3  | 2.42                     | 0.50              |
| 16:CP:49:LEU:HD11  | 16:CP:51:VAL:CG2  | 2.42                     | 0.50              |
| 19:CS:6:LYS:HD3    | 19:CS:7:LYS:HE2   | 1.93                     | 0.50              |
| 20:CT:85:MET:C     | 20:CT:87:LYS:N    | 2.64                     | 0.50              |
| 20:CT:90:GLN:O     | 20:CT:91:LEU:HD23 | 2.11                     | 0.50              |
| 55:D6:43:CYS:O     | 55:D6:43:CYS:SG   | 2.70                     | 0.50              |
| 27:DA:1603:A:C2    | 27:DA:1604:C:C2   | 3.00                     | 0.50              |
| 27:DA:1914:C:H2'   | 27:DA:1915:U:C6   | 2.46                     | 0.50              |
| 27:DA:1952:A:N6    | 27:DA:1953:A:N6   | 2.59                     | 0.50              |
| 27:DA:2196:C:H2'   | 27:DA:2197:U:H6   | 1.76                     | 0.50              |
| 27:DA:2447:G:C4    | 27:DA:2501:C:C5   | 3.00                     | 0.50              |
| 27:DA:475:U:O2'    | 27:DA:476:G:C8    | 2.53                     | 0.50              |
| 27:DA:696:G:N2     | 27:DA:697:C:H1'   | 2.26                     | 0.50              |
| 27:DA:714:U:O2     | 27:DA:717:G:H8    | 1.94                     | 0.50              |
| 27:DA:935:C:H2'    | 27:DA:936:C:H6    | 1.76                     | 0.50              |
| 29:DC:36:LYS:CB    | 29:DC:36:LYS:HZ3  | 2.20                     | 0.50              |
| 27:DA:2636:U:OP1   | 31:DE:80:GLU:HB2  | 2.10                     | 0.50              |
| 31:DE:84:PHE:HE2   | 31:DE:86:PRO:HB3  | 1.76                     | 0.50              |
| 32:DF:170:LEU:HD21 | 32:DF:172:TRP:CE2 | 2.47                     | 0.50              |
| 33:DG:141:PHE:CB   | 33:DG:142:PRO:HD2 | 2.42                     | 0.50              |
| 34:DH:20:ALA:HB3   | 34:DH:23:ARG:HB2  | 1.93                     | 0.50              |
| 34:DH:68:THR:HG23  | 34:DH:72:ILE:HD11 | 1.94                     | 0.50              |
| 35:DI:110:ASP:O    | 35:DI:112:LYS:N   | 2.35                     | 0.50              |
| 40:DR:63:ARG:HG3   | 40:DR:63:ARG:HH11 | 1.76                     | 0.50              |
| 40:DR:94:TYR:CD1   | 40:DR:94:TYR:N    | 2.79                     | 0.50              |
| 28:DB:29:A:OP2     | 41:DS:32:LEU:HG   | 2.11                     | 0.50              |
| 44:DV:19:LYS:HZ3   | 44:DV:20:LEU:N    | 2.09                     | 0.50              |
| 47:DY:2:ARG:O      | 47:DY:3:VAL:HB    | 2.11                     | 0.50              |
| 1:AA:1278:U:H5''   | 1:AA:1279:A:O4'   | 2.11                     | 0.50              |
| 1:AA:235:C:H5'     | 17:AQ:70:ARG:HG2  | 1.94                     | 0.50              |
| 1:AA:259:G:H2'     | 1:AA:260:G:C8     | 2.45                     | 0.50              |
| 1:AA:986:A:H2'     | 1:AA:987:G:H8     | 1.77                     | 0.50              |
| 2:AB:239:VAL:HG12  | 2:AB:239:VAL:O    | 2.11                     | 0.50              |
| 1:AA:1205:U:H4'    | 3:AC:195:VAL:HG22 | 1.94                     | 0.50              |
| 5:AE:145:LYS:O     | 5:AE:148:VAL:HB   | 2.11                     | 0.50              |
| 5:AE:48:ALA:HB3    | 5:AE:54:ALA:HB2   | 1.94                     | 0.50              |
| 6:AF:44:GLY:HA2    | 6:AF:59:TYR:CD2   | 2.47                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:939:G:H5''    | 7:AG:102:ARG:NH2  | 2.26                     | 0.50              |
| 10:AJ:83:GLU:C     | 10:AJ:85:LEU:H    | 2.15                     | 0.50              |
| 11:AK:21:ILE:HG13  | 11:AK:30:VAL:CG1  | 2.42                     | 0.50              |
| 16:AP:75:ARG:C     | 16:AP:77:ALA:H    | 2.14                     | 0.50              |
| 23:AW:42:G:C2'     | 23:AW:43:C:H5''   | 2.41                     | 0.50              |
| 50:B1:5:CYS:SG     | 50:B1:8:SER:OG    | 2.58                     | 0.50              |
| 57:B8:21:LYS:CD    | 57:B8:48:PHE:CZ   | 2.94                     | 0.50              |
| 27:BA:1279:G:C2    | 27:BA:1292:U:C2   | 2.99                     | 0.50              |
| 27:BA:1338:G:H2'   | 27:BA:1339:G:C8   | 2.46                     | 0.50              |
| 27:BA:142:A:H1'    | 27:BA:1408:C:O4'  | 2.12                     | 0.50              |
| 27:BA:1447:G:H2'   | 27:BA:1448:G:C8   | 2.41                     | 0.50              |
| 27:BA:1466:G:H2'   | 27:BA:1547:C:N4   | 2.27                     | 0.50              |
| 27:BA:1721:G:C6    | 27:BA:1739:U:H5'  | 2.45                     | 0.50              |
| 27:BA:1799:G:C2    | 27:BA:1819:A:N7   | 2.79                     | 0.50              |
| 27:BA:1991:U:C5'   | 27:BA:1991:U:H6   | 2.24                     | 0.50              |
| 27:BA:2093:G:C6    | 27:BA:2225:A:C8   | 3.00                     | 0.50              |
| 27:BA:2439:A:H1'   | 27:BA:2587:A:OP1  | 2.12                     | 0.50              |
| 27:BA:271(U):G:C2  | 27:BA:271(V):G:C8 | 3.00                     | 0.50              |
| 27:BA:373:U:O2     | 27:BA:423:A:C2    | 2.64                     | 0.50              |
| 27:BA:524:U:H4'    | 27:BA:555:U:H4'   | 1.93                     | 0.50              |
| 30:BD:31:LYS:HE2   | 30:BD:94:LEU:HD11 | 1.93                     | 0.50              |
| 30:BD:35:LYS:N     | 30:BD:36:PRO:CD   | 2.68                     | 0.50              |
| 31:BE:102:VAL:HG12 | 31:BE:199:ARG:O   | 2.10                     | 0.50              |
| 32:BF:179:GLU:OE2  | 32:BF:179:GLU:N   | 2.38                     | 0.50              |
| 32:BF:65:TRP:HB3   | 32:BF:66:PRO:CD   | 2.40                     | 0.50              |
| 33:BG:135:LEU:HD13 | 33:BG:155:MET:HG3 | 1.94                     | 0.50              |
| 37:BO:4:PRO:O      | 37:BO:5:GLN:CB    | 2.59                     | 0.50              |
| 38:BP:96:THR:HB    | 38:BP:97:PRO:CD   | 2.42                     | 0.50              |
| 44:BV:15:GLU:O     | 44:BV:17:GLY:N    | 2.45                     | 0.50              |
| 43:BU:95:LEU:HD22  | 44:BV:4:ILE:HD11  | 1.93                     | 0.50              |
| 44:BV:5:VAL:HG23   | 44:BV:6:LYS:N     | 2.26                     | 0.50              |
| 1:CA:1362:C:O2     | 1:CA:1363:C:C5    | 2.65                     | 0.50              |
| 1:CA:14:U:C6       | 1:CA:16:A:OP2     | 2.65                     | 0.50              |
| 1:CA:216:G:C5      | 1:CA:217:C:N4     | 2.80                     | 0.50              |
| 1:CA:801:U:O2'     | 1:CA:802:A:H5'    | 2.11                     | 0.50              |
| 2:CB:164:VAL:HG12  | 2:CB:166:ASP:H    | 1.76                     | 0.50              |
| 2:CB:231:GLU:O     | 2:CB:231:GLU:HG3  | 2.11                     | 0.50              |
| 3:CC:196:LEU:HD12  | 3:CC:197:GLY:H    | 1.77                     | 0.50              |
| 4:CD:70:ILE:HD12   | 4:CD:100:ARG:CD   | 2.42                     | 0.50              |
| 4:CD:4:TYR:O       | 4:CD:5:ILE:HB     | 2.10                     | 0.50              |
| 5:CE:26:PHE:N      | 5:CE:26:PHE:CD1   | 2.80                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:33:VAL:HG12   | 5:CE:34:VAL:H      | 1.75                     | 0.50              |
| 5:CE:50:GLU:HG3    | 5:CE:51:VAL:H      | 1.76                     | 0.50              |
| 5:CE:94:ALA:HB3    | 5:CE:117:ASP:C     | 2.32                     | 0.50              |
| 7:CG:77:SER:O      | 7:CG:78:ARG:HB2    | 2.11                     | 0.50              |
| 11:CK:32:ILE:HG12  | 11:CK:41:THR:O     | 2.12                     | 0.50              |
| 12:CL:107:VAL:HG23 | 12:CL:117:TYR:HB3  | 1.92                     | 0.50              |
| 14:CN:34:TYR:CD1   | 14:CN:34:TYR:N     | 2.80                     | 0.50              |
| 18:CR:26:LEU:HD21  | 18:CR:42:ARG:HD2   | 1.93                     | 0.50              |
| 18:CR:66:LEU:HD11  | 18:CR:70:ILE:HD11  | 1.94                     | 0.50              |
| 20:CT:20:LEU:O     | 20:CT:21:LYS:C     | 2.50                     | 0.50              |
| 22:CV:9:G:N7       | 22:CV:10:U:C5      | 2.80                     | 0.50              |
| 23:CW:38:U:H2'     | 23:CW:39:C:C6      | 2.47                     | 0.50              |
| 25:CY:18:G:C1'     | 25:CY:56:G:H22     | 2.23                     | 0.50              |
| 25:CY:27:C:H2'     | 25:CY:28:G:C8      | 2.47                     | 0.50              |
| 57:D8:61:LEU:C     | 57:D8:63:PRO:HD2   | 2.32                     | 0.50              |
| 27:DA:1204:A:N1    | 27:DA:1241:A:H2    | 2.08                     | 0.50              |
| 27:DA:1275:A:H4'   | 27:DA:1276:A:OP1   | 2.12                     | 0.50              |
| 27:DA:1889:A:C6    | 27:DA:1890:A:C5    | 3.00                     | 0.50              |
| 27:DA:1889:A:H2'   | 27:DA:1890:A:O4'   | 2.10                     | 0.50              |
| 27:DA:1902:C:O2'   | 30:DD:244:ARG:HB2  | 2.11                     | 0.50              |
| 27:DA:1931:U:O2'   | 27:DA:1932:A:H5'   | 2.11                     | 0.50              |
| 27:DA:1980:G:H4'   | 27:DA:1981:A:OP2   | 2.11                     | 0.50              |
| 27:DA:2016:U:O2    | 54:D5:7:PRO:HG2    | 2.11                     | 0.50              |
| 27:DA:1669:A:O2'   | 27:DA:2549:G:OP1   | 2.29                     | 0.50              |
| 27:DA:2551:C:H2'   | 27:DA:2552:U:C5    | 2.46                     | 0.50              |
| 27:DA:2824:C:C5    | 27:DA:2825:C:C4    | 3.00                     | 0.50              |
| 27:DA:304:G:O2'    | 27:DA:305:U:H5'    | 2.12                     | 0.50              |
| 27:DA:336:C:O2'    | 27:DA:337:C:H5'    | 2.12                     | 0.50              |
| 27:DA:503:A:C6     | 27:DA:506:G:C6     | 2.99                     | 0.50              |
| 27:DA:99:U:O2      | 27:DA:99:U:H3'     | 2.12                     | 0.50              |
| 28:DB:29:A:H2'     | 28:DB:30:C:C6      | 2.47                     | 0.50              |
| 30:DD:182:LEU:CB   | 30:DD:271:ILE:HG13 | 2.42                     | 0.50              |
| 30:DD:87:ASN:O     | 30:DD:88:ARG:HB3   | 2.11                     | 0.50              |
| 31:DE:117:MET:SD   | 31:DE:136:ARG:HA   | 2.51                     | 0.50              |
| 31:DE:4:ILE:HD11   | 31:DE:31:CYS:SG    | 2.52                     | 0.50              |
| 35:DI:9:LEU:O      | 35:DI:13:GLY:HA3   | 2.11                     | 0.50              |
| 35:DI:7:GLU:OE1    | 35:DI:8:PRO:HD2    | 2.11                     | 0.50              |
| 36:DN:16:ILE:HG23  | 36:DN:54:VAL:HA    | 1.94                     | 0.50              |
| 27:DA:662:G:H5'    | 38:DP:18:ARG:CA    | 2.41                     | 0.50              |
| 39:DQ:29:PHE:HB2   | 39:DQ:105:GLU:OE2  | 2.11                     | 0.50              |
| 39:DQ:114:ALA:O    | 39:DQ:115:MET:C    | 2.50                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DS:24:LEU:HB3  | 41:DS:85:VAL:CG1  | 2.24                     | 0.50              |
| 41:DS:31:SER:O    | 41:DS:33:LYS:N    | 2.44                     | 0.50              |
| 42:DT:28:VAL:HG11 | 42:DT:46:GLU:HG3  | 1.93                     | 0.50              |
| 45:DW:18:ARG:C    | 45:DW:20:VAL:N    | 2.65                     | 0.50              |
| 1:AA:100:C:H2'    | 1:AA:101:A:H8     | 1.67                     | 0.50              |
| 1:AA:1255:G:OP1   | 10:AJ:45:ARG:NH2  | 2.45                     | 0.50              |
| 1:AA:1367:C:N3    | 1:AA:1368:G:C8    | 2.80                     | 0.50              |
| 1:AA:232:G:C4     | 1:AA:233:C:C6     | 2.99                     | 0.50              |
| 1:AA:60:A:C4'     | 1:AA:61:G:O5'     | 2.57                     | 0.50              |
| 1:AA:660:G:H2'    | 1:AA:661:G:C8     | 2.47                     | 0.50              |
| 1:AA:712:A:H2'    | 1:AA:713:G:C8     | 2.47                     | 0.50              |
| 1:AA:943:U:C4     | 1:AA:944:G:N7     | 2.80                     | 0.50              |
| 2:AB:73:THR:HG23  | 2:AB:170:GLU:HG2  | 1.94                     | 0.50              |
| 2:AB:182:ILE:O    | 2:AB:183:PRO:C    | 2.50                     | 0.50              |
| 4:AD:119:GLN:NE2  | 4:AD:123:HIS:NE2  | 2.58                     | 0.50              |
| 5:AE:91:LEU:CD1   | 5:AE:120:THR:HG22 | 2.40                     | 0.50              |
| 5:AE:18:ARG:HG3   | 5:AE:25:ARG:O     | 2.12                     | 0.50              |
| 8:AH:26:VAL:HG23  | 8:AH:27:PRO:HD2   | 1.94                     | 0.50              |
| 10:AJ:33:GLN:O    | 10:AJ:75:ILE:HG23 | 2.12                     | 0.50              |
| 15:AO:76:GLU:OE2  | 15:AO:76:GLU:HA   | 2.12                     | 0.50              |
| 21:AU:7:ARG:O     | 21:AU:8:THR:HG22  | 2.12                     | 0.50              |
| 27:BA:2230:G:H1'  | 50:B1:45:ASN:ND2  | 2.27                     | 0.50              |
| 51:B2:15:LYS:C    | 51:B2:16:LEU:HD23 | 2.32                     | 0.50              |
| 55:B6:15:GLU:HG2  | 55:B6:18:ARG:CZ   | 2.42                     | 0.50              |
| 55:B6:8:LYS:O     | 55:B6:9:LEU:HB3   | 2.11                     | 0.50              |
| 27:BA:1144:G:H2'  | 27:BA:1145:C:C6   | 2.46                     | 0.50              |
| 27:BA:1166:C:H2'  | 27:BA:1167:U:C6   | 2.47                     | 0.50              |
| 27:BA:132:G:H2'   | 27:BA:133:C:H6    | 1.77                     | 0.50              |
| 27:BA:1353:A:H4'  | 30:BD:38:LYS:CE   | 2.36                     | 0.50              |
| 27:BA:1381:G:O2'  | 27:BA:1382:G:H5'  | 2.12                     | 0.50              |
| 27:BA:1526:G:C6   | 27:BA:1527:G:C2   | 2.99                     | 0.50              |
| 27:BA:1565:C:H1'  | 27:BA:1566:A:H2'  | 1.93                     | 0.50              |
| 27:BA:1627:G:H2'  | 27:BA:1628:G:H8   | 1.77                     | 0.50              |
| 27:BA:1936:A:H3'  | 27:BA:1937:A:C5'  | 2.42                     | 0.50              |
| 27:BA:1658:C:H42  | 27:BA:2002:G:H1   | 1.60                     | 0.50              |
| 27:BA:2114:A:O5'  | 27:BA:2114:A:H8   | 1.94                     | 0.50              |
| 27:BA:2158:A:H4'  | 27:BA:2159:G:O5'  | 2.12                     | 0.50              |
| 27:BA:2291:U:H2'  | 27:BA:2292:C:C6   | 2.46                     | 0.50              |
| 27:BA:460:A:C2    | 27:BA:461:C:H1'   | 2.47                     | 0.50              |
| 27:BA:660:G:O2'   | 27:BA:661:C:H5'   | 2.12                     | 0.50              |
| 27:BA:942:G:H2'   | 27:BA:943:U:H5'   | 1.92                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BD:78:LYS:HG2  | 30:BD:79:VAL:H     | 1.77                     | 0.50              |
| 32:BF:175:THR:CG2 | 32:BF:175:THR:O    | 2.59                     | 0.50              |
| 32:BF:46:ARG:O    | 32:BF:48:THR:N     | 2.45                     | 0.50              |
| 33:BG:166:ASP:O   | 33:BG:167:GLU:C    | 2.50                     | 0.50              |
| 33:BG:166:ASP:O   | 33:BG:169:ALA:HB3  | 2.12                     | 0.50              |
| 33:BG:118:ARG:N   | 33:BG:181:ARG:HH21 | 2.00                     | 0.50              |
| 34:BH:153:LYS:HD2 | 34:BH:153:LYS:H    | 1.77                     | 0.50              |
| 35:BI:4:ILE:HG12  | 35:BI:18:VAL:HG22  | 1.93                     | 0.50              |
| 36:BN:57:ALA:C    | 36:BN:58:ASP:O     | 2.50                     | 0.50              |
| 36:BN:95:PRO:HG2  | 36:BN:96:GLU:OE2   | 2.11                     | 0.50              |
| 39:BQ:18:LYS:O    | 39:BQ:19:GLY:O     | 2.30                     | 0.50              |
| 42:BT:54:ARG:O    | 42:BT:55:ASN:HB2   | 2.11                     | 0.50              |
| 47:BY:2:ARG:HD3   | 47:BY:2:ARG:C      | 2.32                     | 0.50              |
| 1:CA:1073:U:OP2   | 5:CE:57:LYS:HE3    | 2.11                     | 0.50              |
| 1:CA:163:C:H2'    | 1:CA:164:U:H6      | 1.75                     | 0.50              |
| 1:CA:486:U:H2'    | 1:CA:487:A:H8      | 1.77                     | 0.50              |
| 1:CA:518:C:OP2    | 1:CA:530:G:H4'     | 2.11                     | 0.50              |
| 3:CC:173:VAL:HG12 | 3:CC:175:LEU:HD12  | 1.93                     | 0.50              |
| 4:CD:154:ASN:C    | 4:CD:155:LEU:HD23  | 2.31                     | 0.50              |
| 4:CD:3:ARG:NH2    | 4:CD:5:ILE:HD11    | 2.27                     | 0.50              |
| 7:CG:76:ARG:HH11  | 7:CG:76:ARG:HG2    | 1.76                     | 0.50              |
| 10:CJ:4:ILE:HB    | 10:CJ:74:ILE:CG1   | 2.41                     | 0.50              |
| 11:CK:21:ILE:HG23 | 11:CK:30:VAL:HG12  | 1.94                     | 0.50              |
| 13:CM:49:THR:HG22 | 13:CM:50:GLU:N     | 2.27                     | 0.50              |
| 1:CA:452:A:N3     | 16:CP:72:ARG:NH1   | 2.59                     | 0.50              |
| 52:D3:8:LEU:HD22  | 52:D3:31:LEU:CD2   | 2.41                     | 0.50              |
| 55:D6:20:ASN:CG   | 55:D6:21:TYR:N     | 2.65                     | 0.50              |
| 27:DA:1582:C:O2'  | 27:DA:1586:A:H8    | 1.94                     | 0.50              |
| 27:DA:1842:G:H2'  | 27:DA:1843:C:C6    | 2.47                     | 0.50              |
| 27:DA:2063:C:C6   | 27:DA:2064:C:C5    | 2.99                     | 0.50              |
| 27:DA:2140:C:H1'  | 27:DA:2152:G:H22   | 1.77                     | 0.50              |
| 27:DA:2382:G:H3'  | 27:DA:2382:G:OP1   | 2.12                     | 0.50              |
| 27:DA:2392:A:OP1  | 57:D8:32:LEU:HD22  | 2.11                     | 0.50              |
| 27:DA:2406:U:C4   | 38:DP:72:PRO:HD2   | 2.47                     | 0.50              |
| 27:DA:560:C:H4'   | 43:DU:52:ARG:CZ    | 2.42                     | 0.50              |
| 27:DA:603:A:H4'   | 27:DA:604:G:O5'    | 2.11                     | 0.50              |
| 27:DA:81:G:H21    | 47:DY:2:ARG:CZ     | 2.24                     | 0.50              |
| 27:DA:849:A:H8    | 27:DA:849:A:O5'    | 1.95                     | 0.50              |
| 27:DA:890:A:OP1   | 27:DA:890:A:H4'    | 2.12                     | 0.50              |
| 28:DB:25:A:H2'    | 28:DB:26:A:C8      | 2.47                     | 0.50              |
| 30:DD:132:PRO:HD3 | 30:DD:190:TYR:CZ   | 2.46                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:DD:53:PHE:CE2  | 30:DD:220:HIS:CD2  | 3.00                     | 0.50              |
| 31:DE:203:LYS:HE3 | 31:DE:204:ALA:N    | 2.27                     | 0.50              |
| 31:DE:40:GLU:OE2  | 31:DE:41:LYS:HG3   | 2.12                     | 0.50              |
| 33:DG:39:ILE:HD13 | 33:DG:157:ILE:HG22 | 1.93                     | 0.50              |
| 33:DG:27:ASN:O    | 33:DG:29:TRP:N     | 2.43                     | 0.50              |
| 34:DH:143:GLN:NE2 | 34:DH:147:ASN:HD21 | 2.10                     | 0.50              |
| 37:DO:86:ILE:CG2  | 37:DO:94:ARG:HD2   | 2.42                     | 0.50              |
| 38:DP:131:SER:O   | 38:DP:133:SER:N    | 2.45                     | 0.50              |
| 38:DP:16:ARG:HD3  | 38:DP:16:ARG:C     | 2.32                     | 0.50              |
| 27:DA:2495:G:OP2  | 39:DQ:82:ARG:NH2   | 2.45                     | 0.50              |
| 1:CA:346:G:H5''   | 42:DT:41:ARG:HH22  | 1.77                     | 0.50              |
| 42:DT:92:GLY:H    | 42:DT:116:ALA:HA   | 1.76                     | 0.50              |
| 44:DV:59:ALA:HA   | 44:DV:97:LYS:HG2   | 1.92                     | 0.50              |
| 47:DY:31:LEU:HD23 | 47:DY:36:ALA:HB3   | 1.94                     | 0.50              |
| 47:DY:96:ILE:CD1  | 47:DY:99:CYS:CB    | 2.89                     | 0.50              |
| 48:DZ:50:ALA:O    | 48:DZ:51:SER:HB3   | 2.12                     | 0.50              |
| 1:AA:1076:C:N4    | 1:AA:1081:G:H1     | 2.06                     | 0.50              |
| 1:AA:1088:G:C4    | 1:AA:1089:G:C8     | 3.00                     | 0.50              |
| 1:AA:1380:U:H4'   | 1:AA:1381:U:C5'    | 2.41                     | 0.50              |
| 1:AA:1402:C:O2'   | 1:AA:1403:C:H5'    | 2.12                     | 0.50              |
| 1:AA:1525:G:H2'   | 1:AA:1526:G:C8     | 2.46                     | 0.50              |
| 1:AA:235:C:H2'    | 1:AA:236:G:H8      | 1.77                     | 0.50              |
| 1:AA:451:A:H61    | 1:AA:481:G:C5'     | 2.25                     | 0.50              |
| 1:AA:737:A:O2'    | 6:AF:72:VAL:HG11   | 2.11                     | 0.50              |
| 1:AA:762:C:H2'    | 1:AA:763:G:C8      | 2.44                     | 0.50              |
| 1:AA:779:C:N4     | 1:AA:780:A:C6      | 2.80                     | 0.50              |
| 2:AB:107:THR:O    | 2:AB:110:GLN:HG3   | 2.12                     | 0.50              |
| 2:AB:140:HIS:O    | 2:AB:144:ARG:HG2   | 2.12                     | 0.50              |
| 4:AD:138:TYR:HE2  | 4:AD:140:VAL:HA    | 1.77                     | 0.50              |
| 5:AE:11:ILE:HD13  | 5:AE:105:VAL:HA    | 1.94                     | 0.50              |
| 8:AH:33:GLU:C     | 8:AH:35:ILE:N      | 2.65                     | 0.50              |
| 14:AN:27:CYS:HG   | 14:AN:43:CYS:HG    | 1.35                     | 0.50              |
| 18:AR:53:ARG:HH21 | 18:AR:59:SER:HA    | 1.76                     | 0.50              |
| 25:AY:47:C:N3     | 25:AY:58:A:H1'     | 2.27                     | 0.50              |
| 27:BA:2278:A:H5'' | 49:B0:12:ASN:HD22  | 1.77                     | 0.50              |
| 58:B9:14:CYS:O    | 58:B9:15:LYS:CB    | 2.51                     | 0.50              |
| 27:BA:1141:U:O4   | 36:BN:64:GLY:HA3   | 2.12                     | 0.50              |
| 27:BA:114:U:H2'   | 27:BA:114:U:O2     | 2.12                     | 0.50              |
| 27:BA:1240:U:O2'  | 27:BA:1241:A:H5'   | 2.12                     | 0.50              |
| 27:BA:1248:G:H3'  | 27:BA:1249:U:H5''  | 1.93                     | 0.50              |
| 27:BA:1260:G:H2'  | 27:BA:1261:C:C6    | 2.47                     | 0.50              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 27:BA:1293:C:C2  | 27:BA:1294:U:C5    | 3.00                     | 0.50              |
| 27:BA:1332:G:H5' | 27:BA:1333:C:H5    | 1.76                     | 0.50              |
| 27:BA:1374:G:H2' | 27:BA:1375:C:C6    | 2.47                     | 0.50              |
| 27:BA:1630:G:H2' | 27:BA:1631:C:C6    | 2.47                     | 0.50              |
| 27:BA:171:G:O2'  | 27:BA:172:C:C6     | 2.56                     | 0.50              |
| 27:BA:1837:C:O2' | 27:BA:1927:A:N3    | 2.36                     | 0.50              |
| 27:BA:2036:C:O2' | 27:BA:2037:G:C8    | 2.65                     | 0.50              |
| 27:BA:2088:G:H2' | 27:BA:2089:U:C6    | 2.47                     | 0.50              |
| 27:BA:2462:U:H6  | 27:BA:2462:U:O5'   | 1.95                     | 0.50              |
| 27:BA:2728:U:H2' | 27:BA:2729:G:H5'   | 1.93                     | 0.50              |
| 27:BA:676:A:N1   | 27:BA:802:A:N1     | 2.59                     | 0.50              |
| 27:BA:872:A:N6   | 27:BA:906:G:C6     | 2.79                     | 0.50              |
| 27:BA:888:C:H3'  | 27:BA:889:C:C5'    | 2.41                     | 0.50              |
| 30:BD:30:GLU:OE2 | 30:BD:63:ARG:NH2   | 2.44                     | 0.50              |
| 27:BA:1812:A:C1' | 30:BD:46:GLN:HE22  | 2.25                     | 0.50              |
| 33:BG:99:MET:O   | 33:BG:103:LEU:HD12 | 2.12                     | 0.50              |
| 35:BI:93:THR:O   | 35:BI:94:ALA:C     | 2.49                     | 0.50              |
| 36:BN:4:TYR:CG   | 43:BU:64:ARG:NH2   | 2.66                     | 0.50              |
| 40:BR:21:TYR:OH  | 40:BR:43:GLU:HG2   | 2.12                     | 0.50              |
| 42:BT:130:ALA:O  | 42:BT:131:ALA:C    | 2.51                     | 0.50              |
| 43:BU:91:ASP:CG  | 43:BU:96:ALA:HB2   | 2.31                     | 0.50              |
| 1:CA:1027:C:C2   | 1:CA:1028:C:N4     | 2.80                     | 0.50              |
| 1:CA:1104:G:H4'  | 2:CB:111:ARG:NH1   | 2.26                     | 0.50              |
| 1:CA:1394:A:O2'  | 1:CA:1501:C:H1'    | 2.11                     | 0.50              |
| 1:CA:598:U:H2'   | 1:CA:599:C:C6      | 2.46                     | 0.50              |
| 1:CA:717:C:C4    | 1:CA:734:G:N7      | 2.80                     | 0.50              |
| 1:CA:757:U:O2'   | 1:CA:758:G:H5'     | 2.11                     | 0.50              |
| 1:CA:810:C:O2'   | 1:CA:811:C:H5'     | 2.12                     | 0.50              |
| 1:CA:889:A:H1'   | 1:CA:891:U:C5      | 2.47                     | 0.50              |
| 2:CB:142:LEU:O   | 2:CB:146:GLN:N     | 2.38                     | 0.50              |
| 2:CB:193:ASP:O   | 2:CB:194:PRO:O     | 2.29                     | 0.50              |
| 3:CC:21:ARG:C    | 3:CC:22:TRP:CD1    | 2.85                     | 0.50              |
| 9:CI:16:ARG:HE   | 9:CI:64:THR:CG2    | 2.24                     | 0.50              |
| 10:CJ:83:GLU:C   | 10:CJ:85:LEU:H     | 2.13                     | 0.50              |
| 15:CO:34:LEU:O   | 15:CO:34:LEU:HD12  | 2.11                     | 0.50              |
| 18:CR:79:LEU:HB3 | 18:CR:80:PRO:HD2   | 1.93                     | 0.50              |
| 20:CT:28:ALA:C   | 20:CT:30:LYS:N     | 2.65                     | 0.50              |
| 23:CW:29:G:H2'   | 23:CW:30:A:H8      | 1.76                     | 0.50              |
| 25:CY:5:G:O2'    | 25:CY:6:U:H5'      | 2.12                     | 0.50              |
| 50:D1:80:LEU:HB3 | 50:D1:82:LEU:CD2   | 2.42                     | 0.50              |
| 50:D1:84:GLY:O   | 50:D1:86:SER:N     | 2.45                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 58:D9:13:LYS:HD3  | 58:D9:28:GLU:HB2   | 1.94                     | 0.50              |
| 27:DA:1171:G:H3'  | 27:DA:1173:G:H4'   | 1.93                     | 0.50              |
| 27:DA:1236:G:OP2  | 27:DA:1236:G:C8    | 2.65                     | 0.50              |
| 27:DA:1311:G:O2'  | 27:DA:1312:U:H5    | 1.95                     | 0.50              |
| 27:DA:1566:A:N7   | 30:DD:214:TRP:CZ3  | 2.80                     | 0.50              |
| 27:DA:23:G:C2     | 27:DA:24:G:C8      | 3.00                     | 0.50              |
| 27:DA:2612:C:HO2' | 27:DA:2613:U:H5'   | 1.76                     | 0.50              |
| 27:DA:284:U:O2'   | 27:DA:285:C:C6     | 2.64                     | 0.50              |
| 27:DA:300:A:N3    | 27:DA:319:C:H1'    | 2.26                     | 0.50              |
| 27:DA:421:U:O2'   | 27:DA:422:A:OP2    | 2.27                     | 0.50              |
| 27:DA:515:A:O2'   | 27:DA:516:C:H5'    | 2.12                     | 0.50              |
| 27:DA:768:G:C6    | 27:DA:769:G:C6     | 2.99                     | 0.50              |
| 27:DA:684:G:O2'   | 27:DA:788:A:N7     | 2.45                     | 0.50              |
| 27:DA:861:A:O2'   | 27:DA:862:G:H5'    | 2.12                     | 0.50              |
| 27:DA:910:A:H3'   | 27:DA:911:A:C8     | 2.45                     | 0.50              |
| 27:DA:972:G:H2'   | 27:DA:973:A:C8     | 2.47                     | 0.50              |
| 27:DA:980:A:H2'   | 27:DA:981:A:O4'    | 2.11                     | 0.50              |
| 30:DD:155:LEU:CD1 | 30:DD:155:LEU:N    | 2.74                     | 0.50              |
| 32:DF:164:ARG:HG2 | 32:DF:164:ARG:HH11 | 1.76                     | 0.50              |
| 32:DF:187:VAL:C   | 38:DP:7:ARG:NH2    | 2.63                     | 0.50              |
| 36:DN:134:ARG:N   | 36:DN:135:PRO:HD3  | 2.26                     | 0.50              |
| 39:DQ:89:ASN:OD1  | 39:DQ:89:ASN:N     | 2.44                     | 0.50              |
| 27:DA:2819:G:OP2  | 40:DR:8:ARG:NH1    | 2.45                     | 0.50              |
| 42:DT:109:GLU:O   | 42:DT:112:ARG:HB2  | 2.12                     | 0.50              |
| 45:DW:84:ARG:CG   | 45:DW:98:LYS:HZ3   | 2.25                     | 0.50              |
| 47:DY:8:LYS:HD2   | 47:DY:8:LYS:N      | 2.26                     | 0.50              |
| 48:DZ:28:TYR:O    | 48:DZ:29:ASN:HB3   | 2.12                     | 0.50              |
| 1:AA:1413:A:C6    | 1:AA:1414:U:C4     | 3.00                     | 0.50              |
| 1:AA:230:G:H4'    | 16:AP:23:ASP:OD2   | 2.11                     | 0.50              |
| 1:AA:800:G:HO2'   | 1:AA:801:U:H6      | 1.56                     | 0.50              |
| 1:AA:818:G:C3'    | 1:AA:819:A:C5'     | 2.90                     | 0.50              |
| 1:AA:839:U:H5'    | 1:AA:840:C:C5      | 2.46                     | 0.50              |
| 2:AB:220:ASP:O    | 2:AB:224:GLN:HB2   | 2.12                     | 0.50              |
| 4:AD:3:ARG:HB3    | 4:AD:118:ARG:HE    | 1.77                     | 0.50              |
| 4:AD:90:GLY:HA3   | 4:AD:201:GLN:NE2   | 2.26                     | 0.50              |
| 4:AD:203:VAL:O    | 4:AD:204:ILE:C     | 2.50                     | 0.50              |
| 5:AE:132:ALA:C    | 5:AE:134:ALA:N     | 2.66                     | 0.50              |
| 5:AE:80:ILE:HD11  | 5:AE:142:LEU:HD21  | 1.94                     | 0.50              |
| 7:AG:23:VAL:HG12  | 7:AG:24:THR:N      | 2.27                     | 0.50              |
| 17:AQ:40:LYS:HE2  | 17:AQ:42:TYR:CZ    | 2.47                     | 0.50              |
| 18:AR:58:LEU:HD12 | 18:AR:58:LEU:N     | 2.27                     | 0.50              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:AA:1313:U:OP1   | 19:AS:6:LYS:HG3     | 2.12                     | 0.50              |
| 21:AU:9:ARG:O     | 21:AU:10:ARG:C      | 2.49                     | 0.50              |
| 1:AA:1494:G:O6    | 26:AZ:1:KBE:HAA     | 2.11                     | 0.50              |
| 51:B2:53:LEU:O    | 51:B2:54:LYS:C      | 2.51                     | 0.50              |
| 57:B8:50:LEU:O    | 57:B8:51:ALA:CB     | 2.59                     | 0.50              |
| 27:BA:1048:A:N6   | 27:BA:1054:A:C5     | 2.79                     | 0.50              |
| 27:BA:1193:G:C8   | 27:BA:1193:G:H5'    | 2.44                     | 0.50              |
| 27:BA:187:G:N3    | 27:BA:1365:A:H2     | 2.10                     | 0.50              |
| 27:BA:1385:G:O3'  | 27:BA:1396:U:H5     | 1.94                     | 0.50              |
| 27:BA:1450:G:H2'  | 27:BA:1450(A):C:C5' | 2.42                     | 0.50              |
| 27:BA:1686:C:C2'  | 27:BA:1687:G:H5'    | 2.42                     | 0.50              |
| 27:BA:1695:G:N2   | 27:BA:1696:G:C5     | 2.80                     | 0.50              |
| 27:BA:2111:C:N3   | 27:BA:2147:G:N2     | 2.59                     | 0.50              |
| 27:BA:633:A:N3    | 27:BA:2403:C:H4'    | 2.27                     | 0.50              |
| 27:BA:2590:A:C2   | 27:BA:2605:U:O2     | 2.64                     | 0.50              |
| 27:BA:370:G:H4'   | 27:BA:371:A:OP2     | 2.11                     | 0.50              |
| 27:BA:463:G:N2    | 27:BA:467:G:C5      | 2.80                     | 0.50              |
| 27:BA:458:G:N2    | 27:BA:469:G:H2'     | 2.26                     | 0.50              |
| 27:BA:196:A:C4    | 27:BA:805:G:O6      | 2.64                     | 0.50              |
| 27:BA:83:G:C2     | 27:BA:102:G:O2'     | 2.63                     | 0.50              |
| 30:BD:131:LEU:O   | 30:BD:190:TYR:HA    | 2.12                     | 0.50              |
| 30:BD:17:THR:HG1  | 30:BD:205:VAL:H     | 1.59                     | 0.50              |
| 30:BD:270:ILE:C   | 30:BD:270:ILE:HD12  | 2.33                     | 0.50              |
| 32:BF:33:LEU:HD13 | 32:BF:112:MET:HE2   | 1.93                     | 0.50              |
| 38:BP:86:LYS:HB2  | 38:BP:117:GLU:O     | 2.11                     | 0.50              |
| 27:BA:814:C:N4    | 38:BP:27:HIS:HD2    | 1.99                     | 0.50              |
| 44:BV:20:LEU:N    | 44:BV:20:LEU:HD12   | 2.27                     | 0.50              |
| 44:BV:82:ARG:NH1  | 44:BV:82:ARG:HG2    | 2.27                     | 0.50              |
| 44:BV:95:LEU:HD22 | 44:BV:95:LEU:C      | 2.33                     | 0.50              |
| 48:BZ:165:SER:HB2 | 48:BZ:166:PRO:C     | 2.32                     | 0.50              |
| 48:BZ:32:LEU:HG   | 48:BZ:33:ASN:N      | 2.27                     | 0.50              |
| 48:BZ:44:ASP:O    | 48:BZ:46:VAL:N      | 2.45                     | 0.50              |
| 1:CA:1003:G:H2'   | 1:CA:1004:A:O4'     | 2.10                     | 0.50              |
| 1:CA:1363:C:H5'   | 1:CA:1363(A):A:P    | 2.52                     | 0.50              |
| 1:CA:487:A:O2'    | 1:CA:488:C:H5'      | 2.11                     | 0.50              |
| 1:CA:604:G:C6     | 1:CA:635:G:C6       | 3.00                     | 0.50              |
| 1:CA:720:C:O5'    | 1:CA:720:C:H6       | 1.94                     | 0.50              |
| 1:CA:885:G:N3     | 1:CA:914:A:H2       | 2.08                     | 0.50              |
| 2:CB:170:GLU:O    | 2:CB:173:ALA:HB3    | 2.12                     | 0.50              |
| 2:CB:58:ILE:N     | 2:CB:58:ILE:HD13    | 2.27                     | 0.50              |
| 3:CC:178:LEU:HD22 | 3:CC:178:LEU:H      | 1.76                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CC:189:ALA:O    | 3:CC:195:VAL:CG1   | 2.60                     | 0.50              |
| 4:CD:13:ARG:HA    | 4:CD:33:MET:SD     | 2.52                     | 0.50              |
| 4:CD:59:ARG:HA    | 4:CD:59:ARG:NE     | 2.26                     | 0.50              |
| 6:CF:5:GLU:OE1    | 6:CF:62:TRP:HZ2    | 1.95                     | 0.50              |
| 7:CG:117:ALA:O    | 7:CG:120:ILE:N     | 2.44                     | 0.50              |
| 9:CI:105:ASP:OD1  | 9:CI:107:ARG:HD3   | 2.12                     | 0.50              |
| 15:CO:8:LYS:O     | 15:CO:11:VAL:HB    | 2.11                     | 0.50              |
| 16:CP:6:LEU:HD23  | 16:CP:17:TYR:CD2   | 2.47                     | 0.50              |
| 27:DA:1140:C:H5'' | 36:DN:66:LYS:HZ3   | 1.76                     | 0.50              |
| 27:DA:1527:G:H5'' | 27:DA:1528:A:OP1   | 2.12                     | 0.50              |
| 27:DA:1548:C:H2'  | 27:DA:1549:C:C6    | 2.42                     | 0.50              |
| 27:DA:2146:C:H4'  | 27:DA:2147:G:O5'   | 2.12                     | 0.50              |
| 27:DA:2354:G:N2   | 27:DA:2355:C:C2    | 2.80                     | 0.50              |
| 27:DA:553:G:O2'   | 27:DA:554:U:H5'    | 2.11                     | 0.50              |
| 27:DA:61:G:O2'    | 27:DA:62:C:H6      | 1.94                     | 0.50              |
| 30:DD:184:LYS:HG3 | 30:DD:269:PHE:HA   | 1.92                     | 0.50              |
| 30:DD:218:ARG:CB  | 30:DD:219:PRO:CD   | 2.90                     | 0.50              |
| 27:DA:1805:U:H5'' | 30:DD:250:TRP:CG   | 2.47                     | 0.50              |
| 37:DO:14:THR:O    | 37:DO:14:THR:HG22  | 2.12                     | 0.50              |
| 38:DP:101:VAL:CG2 | 38:DP:102:ARG:N    | 2.74                     | 0.50              |
| 38:DP:132:LYS:O   | 38:DP:136:GLU:HG2  | 2.12                     | 0.50              |
| 40:DR:11:ASN:O    | 40:DR:12:ARG:HB2   | 2.12                     | 0.50              |
| 42:DT:13:ARG:HH12 | 42:DT:15:VAL:HG11  | 1.77                     | 0.50              |
| 42:DT:49:VAL:O    | 42:DT:50:ILE:HD12  | 2.12                     | 0.50              |
| 44:DV:21:ARG:N    | 44:DV:21:ARG:HD3   | 2.26                     | 0.50              |
| 44:DV:79:VAL:O    | 44:DV:80:GLN:HB2   | 2.12                     | 0.50              |
| 45:DW:25:ARG:HH11 | 45:DW:25:ARG:CB    | 2.25                     | 0.50              |
| 45:DW:25:ARG:HB2  | 45:DW:25:ARG:NH1   | 2.27                     | 0.50              |
| 45:DW:35:ILE:HG23 | 54:D5:28:PRO:HD2   | 1.94                     | 0.50              |
| 45:DW:6:ILE:HG21  | 45:DW:8:ARG:HG3    | 1.93                     | 0.50              |
| 47:DY:90:LEU:HD12 | 47:DY:91:GLU:N     | 2.27                     | 0.50              |
| 48:DZ:140:VAL:O   | 48:DZ:140:VAL:HG13 | 2.11                     | 0.50              |
| 48:DZ:36:VAL:O    | 48:DZ:37:TYR:HB3   | 2.11                     | 0.50              |
| 1:AA:1089:G:O2'   | 1:AA:1090:U:H5'    | 2.12                     | 0.49              |
| 1:AA:1149:C:O2'   | 1:AA:1150:U:H5'    | 2.12                     | 0.49              |
| 1:AA:1154:G:H2'   | 1:AA:1155:G:C8     | 2.46                     | 0.49              |
| 1:AA:1234:C:H2'   | 1:AA:1235:U:H6     | 1.77                     | 0.49              |
| 1:AA:1278:U:H5'   | 1:AA:1279:A:N9     | 2.26                     | 0.49              |
| 1:AA:1377:A:H2'   | 7:AG:7:ALA:HB2     | 1.94                     | 0.49              |
| 1:AA:232:G:C5     | 1:AA:233:C:C5      | 3.00                     | 0.49              |
| 1:AA:277:C:P      | 17:AQ:41:LYS:HZ1   | 2.35                     | 0.49              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:AA:530:G:HO2'   | 1:AA:531:U:P        | 2.34                     | 0.49              |
| 1:AA:758:G:H5''   | 1:AA:880:C:H1'      | 1.93                     | 0.49              |
| 1:AA:799:G:C2'    | 1:AA:800:G:H5'      | 2.41                     | 0.49              |
| 1:AA:799:G:H2'    | 1:AA:800:G:H5'      | 1.93                     | 0.49              |
| 1:AA:848:C:O2'    | 1:AA:849:C:H5'      | 2.12                     | 0.49              |
| 1:AA:938:A:O2'    | 1:AA:939:G:H5'      | 2.11                     | 0.49              |
| 2:AB:108:ILE:O    | 2:AB:111:ARG:HB2    | 2.12                     | 0.49              |
| 4:AD:168:ARG:HH11 | 4:AD:168:ARG:CG     | 2.25                     | 0.49              |
| 5:AE:40:ARG:HB3   | 5:AE:66:MET:HE1     | 1.94                     | 0.49              |
| 6:AF:15:ASP:O     | 6:AF:16:GLN:C       | 2.50                     | 0.49              |
| 8:AH:102:ARG:HD2  | 8:AH:105:ARG:HH12   | 1.77                     | 0.49              |
| 8:AH:119:LEU:HD12 | 8:AH:124:ALA:HA     | 1.94                     | 0.49              |
| 11:AK:32:ILE:HD11 | 11:AK:41:THR:CB     | 2.33                     | 0.49              |
| 12:AL:66:TYR:HB2  | 12:AL:93:VAL:HG11   | 1.93                     | 0.49              |
| 13:AM:57:ARG:NH1  | 53:B4:60:GLU:HG3    | 2.27                     | 0.49              |
| 18:AR:56:THR:O    | 18:AR:58:LEU:HD12   | 2.12                     | 0.49              |
| 50:B1:18:ILE:CG2  | 50:B1:20:ARG:HG3    | 2.42                     | 0.49              |
| 27:BA:1009:A:H5'' | 43:BU:63:VAL:CG2    | 2.43                     | 0.49              |
| 27:BA:1055:G:C2'  | 27:BA:1108:U:H5'    | 2.42                     | 0.49              |
| 27:BA:77:C:C2     | 27:BA:110:G:N2      | 2.80                     | 0.49              |
| 27:BA:1450:G:C2'  | 27:BA:1450(A):C:H5' | 2.41                     | 0.49              |
| 27:BA:1582:C:O2'  | 27:BA:1586:A:C8     | 2.65                     | 0.49              |
| 27:BA:1773:A:C2'  | 27:BA:1774:C:H5'    | 2.42                     | 0.49              |
| 27:BA:1789:A:OP1  | 30:BD:222:ARG:HG3   | 2.11                     | 0.49              |
| 27:BA:1973:G:H2'  | 27:BA:1974:C:C6     | 2.44                     | 0.49              |
| 27:BA:2070:G:C2   | 27:BA:2071:A:C4     | 2.99                     | 0.49              |
| 27:BA:2220:G:H2'  | 27:BA:2221:G:C8     | 2.47                     | 0.49              |
| 27:BA:2289:G:H2'  | 27:BA:2290:G:H5''   | 1.93                     | 0.49              |
| 27:BA:1759:A:H1'  | 27:BA:2711:A:C2     | 2.47                     | 0.49              |
| 27:BA:465:G:C6    | 27:BA:466:A:N6      | 2.80                     | 0.49              |
| 27:BA:601:C:O2'   | 27:BA:605:C:OP1     | 2.23                     | 0.49              |
| 27:BA:65:C:O2'    | 27:BA:66:C:H5'      | 2.12                     | 0.49              |
| 27:BA:787:U:H5''  | 27:BA:788:A:C5'     | 2.42                     | 0.49              |
| 27:BA:997:G:OP1   | 43:BU:92:ARG:C      | 2.50                     | 0.49              |
| 28:BB:37:C:H2'    | 28:BB:38:C:O4'      | 2.11                     | 0.49              |
| 30:BD:105:ILE:O   | 30:BD:106:ILE:C     | 2.50                     | 0.49              |
| 30:BD:126:GLN:O   | 30:BD:127:VAL:C     | 2.50                     | 0.49              |
| 30:BD:261:LYS:NZ  | 30:BD:263:ARG:NH2   | 2.60                     | 0.49              |
| 31:BE:40:GLU:N    | 31:BE:40:GLU:CD     | 2.65                     | 0.49              |
| 32:BF:38:ARG:NH1  | 32:BF:38:ARG:HG3    | 2.24                     | 0.49              |
| 32:BF:3:GLU:HA    | 32:BF:24:LEU:CB     | 2.42                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BG:77:ILE:HG22 | 33:BG:80:PHE:H     | 1.77                     | 0.49              |
| 34:BH:138:LYS:N   | 34:BH:141:VAL:HG23 | 2.21                     | 0.49              |
| 36:BN:55:VAL:HG22 | 36:BN:56:ASN:H     | 1.77                     | 0.49              |
| 38:BP:34:GLY:O    | 38:BP:35:HIS:CB    | 2.60                     | 0.49              |
| 43:BU:31:SER:OG   | 43:BU:34:LYS:N     | 2.35                     | 0.49              |
| 43:BU:52:ARG:O    | 43:BU:56:ASP:N     | 2.42                     | 0.49              |
| 44:BV:2:PHE:CE1   | 44:BV:13:ARG:HG3   | 2.46                     | 0.49              |
| 44:BV:38:LEU:HD23 | 44:BV:39:LEU:N     | 2.27                     | 0.49              |
| 47:BY:49:VAL:O    | 47:BY:50:ARG:HB2   | 2.13                     | 0.49              |
| 48:BZ:106:THR:HB  | 48:BZ:107:PRO:HD2  | 1.93                     | 0.49              |
| 1:CA:1016:A:H2'   | 1:CA:1017:G:O4'    | 2.12                     | 0.49              |
| 1:CA:1030:C:C5    | 1:CA:1031:G:N2     | 2.79                     | 0.49              |
| 1:CA:1296:C:H3'   | 1:CA:1297:C:C6     | 2.46                     | 0.49              |
| 1:CA:1382:C:O2'   | 1:CA:1383:C:H5'    | 2.12                     | 0.49              |
| 1:CA:18:C:H2'     | 1:CA:19:C:O4'      | 2.12                     | 0.49              |
| 1:CA:40:C:O2'     | 1:CA:41:G:H5'      | 2.12                     | 0.49              |
| 1:CA:59:A:H5''    | 1:CA:60:A:H5'      | 1.93                     | 0.49              |
| 1:CA:748:C:HO2'   | 1:CA:749:C:P       | 2.35                     | 0.49              |
| 1:CA:77:G:H2'     | 1:CA:77:G:N3       | 2.27                     | 0.49              |
| 1:CA:936:C:H2'    | 1:CA:937:A:O4'     | 2.12                     | 0.49              |
| 4:CD:146:ILE:CD1  | 4:CD:146:ILE:N     | 2.71                     | 0.49              |
| 9:CI:17:VAL:HG12  | 9:CI:17:VAL:O      | 2.11                     | 0.49              |
| 10:CJ:84:GLN:CD   | 10:CJ:84:GLN:H     | 2.14                     | 0.49              |
| 11:CK:24:SER:OG   | 11:CK:25:TYR:N     | 2.42                     | 0.49              |
| 12:CL:49:LEU:O    | 12:CL:51:LYS:HD2   | 2.12                     | 0.49              |
| 15:CO:56:LEU:O    | 15:CO:57:LEU:C     | 2.50                     | 0.49              |
| 16:CP:59:TRP:O    | 16:CP:64:ALA:HB3   | 2.12                     | 0.49              |
| 18:CR:46:GLU:HB3  | 18:CR:85:LEU:HD13  | 1.93                     | 0.49              |
| 1:CA:103:C:OP1    | 20:CT:17:ARG:NH1   | 2.45                     | 0.49              |
| 20:CT:40:ALA:C    | 20:CT:42:GLN:H     | 2.15                     | 0.49              |
| 24:CX:34:C:O2     | 24:CX:35:A:C8      | 2.64                     | 0.49              |
| 50:D1:50:ARG:CG   | 50:D1:50:ARG:HH11  | 2.23                     | 0.49              |
| 56:D7:22:MET:SD   | 56:D7:31:LEU:CD1   | 3.00                     | 0.49              |
| 57:D8:33:ASN:HA   | 57:D8:36:LYS:HD2   | 1.94                     | 0.49              |
| 27:DA:242:G:N7    | 57:D8:5:LYS:HG2    | 2.27                     | 0.49              |
| 58:D9:27:CYS:SG   | 58:D9:29:ASN:ND2   | 2.85                     | 0.49              |
| 27:DA:1400:G:O2'  | 27:DA:1401:G:H5'   | 2.12                     | 0.49              |
| 27:DA:1770:G:H2'  | 27:DA:1771:C:C6    | 2.46                     | 0.49              |
| 27:DA:1823:G:H2'  | 27:DA:1824:G:H8    | 1.77                     | 0.49              |
| 27:DA:1932:A:O2'  | 27:DA:1933:G:H5'   | 2.11                     | 0.49              |
| 27:DA:1952:A:C6   | 27:DA:1953:A:C6    | 3.00                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:2259:G:H1'  | 27:DA:2427:C:C2    | 2.47                     | 0.49              |
| 27:DA:2543:G:C2   | 27:DA:2544:G:C4    | 2.99                     | 0.49              |
| 27:DA:2755:C:H2'  | 27:DA:2755:C:O2    | 2.12                     | 0.49              |
| 27:DA:481:G:O2'   | 27:DA:482:A:P      | 2.70                     | 0.49              |
| 27:DA:811:U:H2'   | 38:DP:24:GLY:O     | 2.12                     | 0.49              |
| 27:DA:869:G:C4    | 27:DA:870:A:C8     | 3.01                     | 0.49              |
| 28:DB:25:A:H3'    | 28:DB:26:A:H5''    | 1.93                     | 0.49              |
| 30:DD:126:GLN:HG2 | 30:DD:129:ASN:ND2  | 2.27                     | 0.49              |
| 31:DE:52:LEU:HD22 | 31:DE:76:ARG:HB2   | 1.94                     | 0.49              |
| 31:DE:96:PHE:HE2  | 31:DE:198:VAL:HG12 | 1.77                     | 0.49              |
| 33:DG:135:LEU:N   | 33:DG:135:LEU:HD12 | 2.25                     | 0.49              |
| 37:DO:88:ASN:ND2  | 37:DO:92:GLU:HB2   | 2.27                     | 0.49              |
| 44:DV:47:VAL:O    | 44:DV:47:VAL:HG23  | 2.12                     | 0.49              |
| 27:DA:1615:C:C2   | 45:DW:87:PRO:HG3   | 2.46                     | 0.49              |
| 46:DX:71:GLY:C    | 46:DX:72:LYS:HD2   | 2.32                     | 0.49              |
| 1:AA:1147:C:O2'   | 9:AI:16:ARG:HD3    | 2.12                     | 0.49              |
| 1:AA:1179:A:H2'   | 1:AA:1180:A:O4'    | 2.12                     | 0.49              |
| 1:AA:1248:A:C2'   | 1:AA:1249:C:H5'    | 2.42                     | 0.49              |
| 1:AA:1342:C:O2'   | 1:AA:1343:G:H5'    | 2.12                     | 0.49              |
| 1:AA:297:G:N2     | 1:AA:300:A:OP2     | 2.39                     | 0.49              |
| 1:AA:806:C:H2'    | 1:AA:807:A:C8      | 2.47                     | 0.49              |
| 1:AA:875:C:H1'    | 8:AH:15:ASN:ND2    | 2.27                     | 0.49              |
| 1:AA:937:A:N6     | 1:AA:938:A:C6      | 2.80                     | 0.49              |
| 2:AB:80:ILE:HD13  | 2:AB:211:ILE:HG22  | 1.92                     | 0.49              |
| 3:AC:200:ALA:C    | 3:AC:201:TYR:HD1   | 2.15                     | 0.49              |
| 8:AH:127:LEU:HD12 | 8:AH:129:VAL:CG1   | 2.38                     | 0.49              |
| 9:AI:43:ALA:HA    | 9:AI:74:ILE:HD13   | 1.94                     | 0.49              |
| 13:AM:22:ILE:HG22 | 13:AM:25:ILE:HD13  | 1.92                     | 0.49              |
| 14:AN:26:ARG:HD2  | 14:AN:43:CYS:SG    | 2.52                     | 0.49              |
| 15:AO:38:ARG:HH11 | 15:AO:38:ARG:CG    | 2.25                     | 0.49              |
| 20:AT:13:LEU:O    | 20:AT:16:HIS:HB3   | 2.12                     | 0.49              |
| 21:AU:12:LYS:HB3  | 21:AU:22:ARG:HD3   | 1.94                     | 0.49              |
| 25:AY:67:C:H2'    | 25:AY:68:C:C6      | 2.45                     | 0.49              |
| 26:AZ:3:SER:O     | 26:AZ:4:SER:HB3    | 2.12                     | 0.49              |
| 51:B2:32:LEU:HB2  | 51:B2:53:LEU:CD1   | 2.42                     | 0.49              |
| 27:BA:125:G:H21   | 56:B7:48:LYS:HZ3   | 1.57                     | 0.49              |
| 27:BA:1338:G:H2'  | 27:BA:1339:G:H8    | 1.77                     | 0.49              |
| 27:BA:153:C:OP1   | 50:B1:92:LYS:HE2   | 2.11                     | 0.49              |
| 27:BA:1602:U:H4'  | 27:BA:1603:A:OP2   | 2.13                     | 0.49              |
| 27:BA:2287:A:C4   | 27:BA:2289:G:N7    | 2.80                     | 0.49              |
| 27:BA:218:A:H2    | 27:BA:235:U:H4'    | 1.75                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2450:A:C2    | 27:BA:2451:A:C4    | 3.00                     | 0.49              |
| 27:BA:271(K):U:H3' | 27:BA:271(L):U:C5' | 2.42                     | 0.49              |
| 27:BA:2817:G:H21   | 27:BA:2836:U:H1'   | 1.78                     | 0.49              |
| 27:BA:2887:U:O2'   | 27:BA:2888:C:H5'   | 2.12                     | 0.49              |
| 27:BA:461:C:O2     | 27:BA:461:C:H2'    | 2.12                     | 0.49              |
| 27:BA:486:C:H2'    | 27:BA:487:C:C6     | 2.47                     | 0.49              |
| 27:BA:511:U:C5     | 27:BA:512:G:C4     | 3.00                     | 0.49              |
| 27:BA:533:G:O2'    | 43:BU:42:ALA:HA    | 2.12                     | 0.49              |
| 27:BA:711:G:N2     | 27:BA:721:C:C2     | 2.79                     | 0.49              |
| 27:BA:886:C:H2'    | 27:BA:889:C:H42    | 1.76                     | 0.49              |
| 27:BA:903:C:H2'    | 27:BA:904:C:C6     | 2.46                     | 0.49              |
| 27:BA:1788:C:H5''  | 30:BD:225:ALA:HB1  | 1.92                     | 0.49              |
| 31:BE:75:VAL:O     | 31:BE:77:ILE:N     | 2.45                     | 0.49              |
| 32:BF:150:GLY:HA2  | 32:BF:172:TRP:CE3  | 2.46                     | 0.49              |
| 33:BG:54:GLU:C     | 33:BG:56:ALA:N     | 2.64                     | 0.49              |
| 34:BH:85:LYS:HB3   | 34:BH:133:VAL:HG23 | 1.92                     | 0.49              |
| 36:BN:1:MET:O      | 36:BN:2:LYS:CG     | 2.61                     | 0.49              |
| 37:BO:22:ILE:HG12  | 37:BO:42:SER:N     | 2.27                     | 0.49              |
| 37:BO:97:ARG:HA    | 37:BO:117:LEU:HD22 | 1.94                     | 0.49              |
| 38:BP:83:VAL:HG22  | 38:BP:83:VAL:O     | 2.12                     | 0.49              |
| 38:BP:85:LEU:HA    | 38:BP:88:LEU:HB2   | 1.94                     | 0.49              |
| 38:BP:96:THR:O     | 38:BP:100:LEU:HD22 | 2.13                     | 0.49              |
| 39:BQ:27:VAL:H     | 39:BQ:137:TYR:HD1  | 1.60                     | 0.49              |
| 47:BY:96:ILE:CG1   | 47:BY:99:CYS:HB2   | 2.43                     | 0.49              |
| 1:CA:1260:C:H6     | 1:CA:1260:C:H3'    | 1.78                     | 0.49              |
| 1:CA:336:C:H2'     | 1:CA:337:C:H5'     | 1.94                     | 0.49              |
| 1:CA:709:G:H2'     | 1:CA:710:G:H8      | 1.76                     | 0.49              |
| 1:CA:925:G:C2      | 1:CA:927:G:C8      | 3.00                     | 0.49              |
| 1:CA:937:A:O5'     | 1:CA:937:A:H8      | 1.95                     | 0.49              |
| 4:CD:100:ARG:O     | 4:CD:101:LEU:C     | 2.50                     | 0.49              |
| 5:CE:50:GLU:HB3    | 5:CE:53:LEU:CD1    | 2.33                     | 0.49              |
| 6:CF:34:GLY:HA3    | 6:CF:71:ARG:HH21   | 1.77                     | 0.49              |
| 6:CF:76:ALA:O      | 6:CF:80:ARG:HG2    | 2.12                     | 0.49              |
| 11:CK:83:ILE:HG12  | 11:CK:109:VAL:HB   | 1.94                     | 0.49              |
| 12:CL:84:GLY:HA2   | 12:CL:95:TYR:HA    | 1.92                     | 0.49              |
| 12:CL:5:ASN:CA     | 12:CL:8:VAL:HG23   | 2.42                     | 0.49              |
| 16:CP:20:VAL:HG22  | 16:CP:21:VAL:H     | 1.76                     | 0.49              |
| 17:CQ:3:LYS:HD3    | 17:CQ:61:GLU:O     | 2.13                     | 0.49              |
| 17:CQ:76:LEU:HD12  | 17:CQ:76:LEU:C     | 2.32                     | 0.49              |
| 1:CA:718:G:N2      | 18:CR:49:LYS:HD3   | 2.27                     | 0.49              |
| 49:D0:14:ARG:O     | 49:D0:15:ASP:HB2   | 2.11                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:D2:30:ARG:O     | 51:D2:31:GLU:C    | 2.51                     | 0.49              |
| 51:D2:4:SER:CA     | 51:D2:7:ARG:HH11  | 2.07                     | 0.49              |
| 27:DA:1545:A:H3'   | 27:DA:1546:C:C6   | 2.47                     | 0.49              |
| 27:DA:18:C:N4      | 27:DA:19:C:N4     | 2.60                     | 0.49              |
| 27:DA:1952:A:H62   | 27:DA:1953:A:N6   | 2.08                     | 0.49              |
| 27:DA:205:G:O2'    | 27:DA:206:U:OP2   | 2.29                     | 0.49              |
| 27:DA:2376:A:H2'   | 27:DA:2377:A:O4'  | 2.11                     | 0.49              |
| 27:DA:2479:G:H5''  | 27:DA:2537:U:H4'  | 1.94                     | 0.49              |
| 27:DA:2712:U:H5''  | 27:DA:2714:G:H4'  | 1.93                     | 0.49              |
| 27:DA:2747:G:O6    | 27:DA:2755:C:H5'' | 2.12                     | 0.49              |
| 27:DA:30:G:C5      | 27:DA:31:C:C4     | 3.00                     | 0.49              |
| 27:DA:330:A:O2'    | 27:DA:331:A:H2'   | 2.12                     | 0.49              |
| 27:DA:434:U:C4'    | 27:DA:435:C:OP1   | 2.55                     | 0.49              |
| 27:DA:746:A:C1'    | 27:DA:748:G:N2    | 2.76                     | 0.49              |
| 27:DA:860:U:O4'    | 27:DA:2268:A:H5'  | 2.13                     | 0.49              |
| 27:DA:953:A:N3     | 27:DA:954:G:C8    | 2.79                     | 0.49              |
| 28:DB:39:A:O2'     | 28:DB:46:A:N1     | 2.41                     | 0.49              |
| 29:DC:52:ARG:HH21  | 29:DC:53:ARG:HH21 | 1.59                     | 0.49              |
| 30:DD:35:LYS:NZ    | 30:DD:104:TYR:H   | 2.08                     | 0.49              |
| 30:DD:176:ARG:HA   | 30:DD:181:GLU:O   | 2.11                     | 0.49              |
| 33:DG:48:GLU:O     | 33:DG:51:ARG:NE   | 2.45                     | 0.49              |
| 33:DG:77:ILE:O     | 33:DG:81:LYS:O    | 2.30                     | 0.49              |
| 36:DN:16:ILE:CG2   | 36:DN:54:VAL:HG23 | 2.42                     | 0.49              |
| 36:DN:78:TYR:HB3   | 36:DN:79:PRO:HD3  | 1.92                     | 0.49              |
| 43:DU:100:VAL:HG12 | 43:DU:101:ARG:HG3 | 1.95                     | 0.49              |
| 48:DZ:9:ARG:HD3    | 48:DZ:11:GLY:HA2  | 1.93                     | 0.49              |
| 1:AA:109:A:C4      | 1:AA:326:G:C2     | 3.00                     | 0.49              |
| 1:AA:128:G:O2'     | 1:AA:129:U:H5'    | 2.12                     | 0.49              |
| 1:AA:220:G:N3      | 1:AA:220:G:H2'    | 2.28                     | 0.49              |
| 1:AA:436:C:H2'     | 1:AA:437:U:C6     | 2.47                     | 0.49              |
| 1:AA:455:C:C2'     | 1:AA:456:C:H5'    | 2.42                     | 0.49              |
| 1:AA:619:U:H3      | 4:AD:135:LEU:HD13 | 1.76                     | 0.49              |
| 1:AA:965:A:H4'     | 1:AA:966:G:H5''   | 1.94                     | 0.49              |
| 2:AB:137:ARG:HD3   | 2:AB:137:ARG:C    | 2.33                     | 0.49              |
| 2:AB:235:SER:HG    | 2:AB:236:TYR:HD1  | 1.60                     | 0.49              |
| 2:AB:67:THR:HG21   | 2:AB:155:LEU:CD2  | 2.42                     | 0.49              |
| 3:AC:73:PRO:O      | 3:AC:75:VAL:N     | 2.44                     | 0.49              |
| 7:AG:103:TRP:HZ3   | 7:AG:138:LYS:HA   | 1.77                     | 0.49              |
| 7:AG:52:GLU:C      | 7:AG:54:THR:H     | 2.16                     | 0.49              |
| 9:AI:48:GLU:C      | 9:AI:50:LEU:N     | 2.63                     | 0.49              |
| 9:AI:73:GLN:O      | 9:AI:76:ALA:HB3   | 2.12                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:AM:116:THR:HG22 | 13:AM:117:VAL:N   | 2.27                     | 0.49              |
| 13:AM:23:TYR:HB3   | 13:AM:67:GLU:HB2  | 1.94                     | 0.49              |
| 14:AN:27:CYS:HG    | 14:AN:40:CYS:HG   | 1.53                     | 0.49              |
| 17:AQ:13:ASP:C     | 17:AQ:15:MET:H    | 2.15                     | 0.49              |
| 19:AS:19:VAL:O     | 19:AS:23:ASN:HB2  | 2.12                     | 0.49              |
| 20:AT:20:LEU:O     | 20:AT:23:ARG:HB3  | 2.12                     | 0.49              |
| 58:B9:27:CYS:CB    | 58:B9:32:HIS:HB2  | 2.42                     | 0.49              |
| 27:BA:1026:U:O2'   | 27:BA:1027:A:H5'  | 2.11                     | 0.49              |
| 27:BA:1710:C:C6    | 27:BA:1710:C:C3'  | 2.95                     | 0.49              |
| 27:BA:188:G:H2'    | 27:BA:189:G:H5'   | 1.93                     | 0.49              |
| 27:BA:2039:C:O2'   | 27:BA:2040:C:H5'  | 2.12                     | 0.49              |
| 27:BA:2093:G:C6    | 27:BA:2225:A:N7   | 2.81                     | 0.49              |
| 27:BA:2251:G:OP2   | 39:BQ:82:ARG:NH1  | 2.46                     | 0.49              |
| 27:BA:2534:A:H2'   | 27:BA:2535:G:O5'  | 2.11                     | 0.49              |
| 27:BA:2657:A:C2'   | 27:BA:2658:C:H5'  | 2.42                     | 0.49              |
| 27:BA:32:C:O2'     | 27:BA:33:U:H5'    | 2.11                     | 0.49              |
| 27:BA:440:G:N2     | 32:BF:46:ARG:HH22 | 2.10                     | 0.49              |
| 27:BA:451:C:C4     | 27:BA:453:C:C5    | 3.01                     | 0.49              |
| 27:BA:638:G:C6     | 27:BA:639:U:C4    | 3.00                     | 0.49              |
| 27:BA:876:C:H2'    | 27:BA:877:U:C6    | 2.47                     | 0.49              |
| 30:BD:70:TRP:HZ3   | 30:BD:146:GLU:CD  | 2.15                     | 0.49              |
| 30:BD:64:ILE:O     | 30:BD:64:ILE:CG2  | 2.58                     | 0.49              |
| 34:BH:44:VAL:C     | 34:BH:46:GLU:H    | 2.15                     | 0.49              |
| 35:BI:6:LEU:O      | 35:BI:7:GLU:C     | 2.51                     | 0.49              |
| 27:BA:671:C:H5     | 38:BP:42:SER:HA   | 1.76                     | 0.49              |
| 39:BQ:38:GLU:HA    | 39:BQ:99:PRO:HG3  | 1.93                     | 0.49              |
| 40:BR:30:THR:HG22  | 40:BR:31:HIS:N    | 2.27                     | 0.49              |
| 43:BU:69:CYS:HB2   | 43:BU:74:LEU:CD1  | 2.39                     | 0.49              |
| 48:BZ:37:TYR:CG    | 48:BZ:37:TYR:O    | 2.64                     | 0.49              |
| 1:CA:1223:C:H5''   | 1:CA:1224:G:H5''  | 1.94                     | 0.49              |
| 1:CA:123:C:H2'     | 1:CA:124:G:O4'    | 2.11                     | 0.49              |
| 1:CA:1269:A:H5''   | 1:CA:1270:C:OP2   | 2.12                     | 0.49              |
| 1:CA:1328:C:P      | 21:CU:21:TYR:OH   | 2.70                     | 0.49              |
| 1:CA:1380:U:H4'    | 1:CA:1381:U:O5'   | 2.12                     | 0.49              |
| 1:CA:422:C:H4'     | 1:CA:423:G:OP1    | 2.11                     | 0.49              |
| 1:CA:296:U:H1'     | 1:CA:556:C:O2'    | 2.12                     | 0.49              |
| 1:CA:601:C:O5'     | 1:CA:601:C:H6     | 1.96                     | 0.49              |
| 1:CA:814:A:H2'     | 1:CA:816:A:H5''   | 1.95                     | 0.49              |
| 1:CA:872:A:C8      | 1:CA:874:G:C8     | 3.00                     | 0.49              |
| 1:CA:891:U:O2'     | 1:CA:892:A:H5'    | 2.12                     | 0.49              |
| 1:CA:949:A:C1'     | 1:CA:1364:U:H3    | 2.25                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CB:114:ARG:HD3   | 2:CB:117:GLU:OE1   | 2.12                     | 0.49              |
| 3:CC:64:VAL:O      | 3:CC:100:ALA:HB3   | 2.13                     | 0.49              |
| 1:CA:1112:C:O2     | 3:CC:179:ARG:HD3   | 2.12                     | 0.49              |
| 6:CF:3:ARG:NH1     | 6:CF:3:ARG:HG3     | 2.22                     | 0.49              |
| 6:CF:93:SER:C      | 6:CF:94:GLN:HG3    | 2.33                     | 0.49              |
| 7:CG:14:PRO:HB3    | 7:CG:19:GLY:O      | 2.12                     | 0.49              |
| 8:CH:113:SER:O     | 8:CH:131:GLY:HA3   | 2.12                     | 0.49              |
| 12:CL:7:LEU:O      | 12:CL:11:GLY:N     | 2.45                     | 0.49              |
| 17:CQ:59:ILE:CG2   | 17:CQ:71:PHE:HB3   | 2.43                     | 0.49              |
| 55:D6:11:LEU:CD1   | 55:D6:52:VAL:O     | 2.56                     | 0.49              |
| 57:D8:62:LEU:N     | 57:D8:63:PRO:HD2   | 2.28                     | 0.49              |
| 57:D8:16:ILE:HG22  | 57:D8:64:TYR:HB3   | 1.94                     | 0.49              |
| 27:DA:1171:G:H5''  | 27:DA:1173:G:H5''  | 1.95                     | 0.49              |
| 27:DA:1289:C:O2'   | 27:DA:1290:C:C6    | 2.62                     | 0.49              |
| 27:DA:1291:C:H2'   | 27:DA:1292:U:C6    | 2.47                     | 0.49              |
| 27:DA:1324:G:C2    | 27:DA:1331:A:C2    | 2.99                     | 0.49              |
| 27:DA:1557:C:H5''  | 27:DA:1558:A:OP2   | 2.12                     | 0.49              |
| 27:DA:1684:C:H2'   | 27:DA:1685:C:C6    | 2.47                     | 0.49              |
| 27:DA:1767:C:C2'   | 27:DA:1768:U:H5'   | 2.41                     | 0.49              |
| 27:DA:20:C:O2'     | 27:DA:21:A:H5'     | 2.12                     | 0.49              |
| 27:DA:2308:G:N7    | 27:DA:2310:A:H5'   | 2.26                     | 0.49              |
| 27:DA:271(A):A:C5' | 27:DA:271(B):C:OP2 | 2.60                     | 0.49              |
| 27:DA:363(E):U:O2  | 27:DA:363(E):U:C2' | 2.59                     | 0.49              |
| 27:DA:534:U:H1'    | 43:DU:49:HIS:CD2   | 2.46                     | 0.49              |
| 27:DA:555:U:O2'    | 27:DA:556:G:H8     | 1.95                     | 0.49              |
| 27:DA:907:U:O2'    | 27:DA:908:C:H5'    | 2.12                     | 0.49              |
| 28:DB:7:G:H3'      | 28:DB:8:U:H5''     | 1.94                     | 0.49              |
| 29:DC:19:VAL:HG12  | 29:DC:20:TYR:HD1   | 1.78                     | 0.49              |
| 31:DE:131:ALA:CB   | 31:DE:134:ILE:HD11 | 2.42                     | 0.49              |
| 33:DG:125:PHE:HD1  | 33:DG:125:PHE:H    | 1.59                     | 0.49              |
| 34:DH:167:GLU:N    | 34:DH:167:GLU:OE1  | 2.45                     | 0.49              |
| 34:DH:84:SER:O     | 34:DH:85:LYS:CB    | 2.60                     | 0.49              |
| 35:DI:110:ASP:O    | 35:DI:114:LEU:HD21 | 2.13                     | 0.49              |
| 37:DO:59:LYS:O     | 37:DO:86:ILE:HA    | 2.13                     | 0.49              |
| 38:DP:113:LYS:O    | 38:DP:115:LEU:HD22 | 2.11                     | 0.49              |
| 38:DP:135:LEU:HD12 | 38:DP:136:GLU:OE1  | 2.13                     | 0.49              |
| 38:DP:50:ARG:NH2   | 38:DP:50:ARG:HG2   | 2.27                     | 0.49              |
| 38:DP:65:ARG:HH11  | 57:D8:46:ARG:NH2   | 2.05                     | 0.49              |
| 38:DP:91:PHE:HD1   | 38:DP:91:PHE:N     | 2.07                     | 0.49              |
| 42:DT:50:ILE:HA    | 42:DT:99:LEU:HD11  | 1.93                     | 0.49              |
| 43:DU:97:ASP:HA    | 43:DU:100:VAL:HG23 | 1.94                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:DU:34:LYS:HE2   | 43:DU:34:LYS:HA   | 1.95                     | 0.49              |
| 43:DU:59:ARG:O     | 43:DU:62:ILE:HB   | 2.12                     | 0.49              |
| 36:DN:42:TRP:CD1   | 43:DU:63:VAL:CG1  | 2.95                     | 0.49              |
| 47:DY:67:LEU:O     | 47:DY:68:HIS:O    | 2.30                     | 0.49              |
| 48:DZ:107:PRO:O    | 48:DZ:109:GLY:N   | 2.45                     | 0.49              |
| 1:AA:994:A:N1      | 1:AA:1047:G:H4'   | 2.27                     | 0.49              |
| 1:AA:1221:G:OP1    | 19:AS:36:ARG:HD3  | 2.13                     | 0.49              |
| 1:AA:1257:U:C6     | 1:AA:1257:U:C3'   | 2.95                     | 0.49              |
| 1:AA:1417:G:N2     | 1:AA:1482:G:H2'   | 2.26                     | 0.49              |
| 1:AA:175:C:H2'     | 1:AA:176:C:H6     | 1.77                     | 0.49              |
| 1:AA:353:A:C2'     | 1:AA:354:G:OP2    | 2.59                     | 0.49              |
| 1:AA:471:G:HO2'    | 1:AA:472:A:H8     | 1.60                     | 0.49              |
| 1:AA:865:A:C2      | 1:AA:918:A:H4'    | 2.47                     | 0.49              |
| 1:AA:1190:G:OP1    | 3:AC:5:ILE:HG13   | 2.12                     | 0.49              |
| 10:AJ:7:LYS:HD3    | 10:AJ:71:LEU:HD13 | 1.94                     | 0.49              |
| 11:AK:80:VAL:O     | 11:AK:80:VAL:HG23 | 2.12                     | 0.49              |
| 12:AL:3:THR:O      | 12:AL:6:GLN:N     | 2.43                     | 0.49              |
| 19:AS:19:VAL:HG13  | 19:AS:47:HIS:CD2  | 2.47                     | 0.49              |
| 55:B6:26:ASN:HB3   | 55:B6:32:ASN:OD1  | 2.13                     | 0.49              |
| 57:B8:39:LYS:O     | 57:B8:43:GLN:HG3  | 2.13                     | 0.49              |
| 27:BA:1159:U:OP1   | 52:B3:30:ARG:NH2  | 2.46                     | 0.49              |
| 27:BA:1777:U:H6    | 27:BA:1777:U:O5'  | 1.95                     | 0.49              |
| 27:BA:2297:C:O5'   | 27:BA:2297:C:H6   | 1.96                     | 0.49              |
| 27:BA:2623:G:H4'   | 27:BA:2825:C:O2   | 2.12                     | 0.49              |
| 27:BA:296:C:N3     | 27:BA:343:C:O2    | 2.45                     | 0.49              |
| 27:BA:662:G:O3'    | 38:BP:20:GLY:HA2  | 2.13                     | 0.49              |
| 28:BB:78:A:C2      | 28:BB:100:A:C4    | 3.00                     | 0.49              |
| 29:BC:193:ILE:C    | 29:BC:195:ALA:N   | 2.66                     | 0.49              |
| 29:BC:64:LEU:O     | 29:BC:66:HIS:N    | 2.39                     | 0.49              |
| 31:BE:1:MET:CB     | 31:BE:84:PHE:HB2  | 2.39                     | 0.49              |
| 32:BF:136:THR:HG22 | 32:BF:166:ALA:O   | 2.13                     | 0.49              |
| 27:BA:1257:C:O2'   | 32:BF:83:PHE:O    | 2.29                     | 0.49              |
| 33:BG:128:ARG:N    | 33:BG:128:ARG:NE  | 2.61                     | 0.49              |
| 39:BQ:81:VAL:CG2   | 39:BQ:82:ARG:N    | 2.76                     | 0.49              |
| 40:BR:34:ILE:CG2   | 40:BR:35:THR:N    | 2.76                     | 0.49              |
| 40:BR:81:ASP:OD2   | 40:BR:81:ASP:N    | 2.45                     | 0.49              |
| 41:BS:88:ASP:O     | 41:BS:89:ARG:O    | 2.31                     | 0.49              |
| 42:BT:28:VAL:CG2   | 42:BT:46:GLU:CA   | 2.86                     | 0.49              |
| 46:BX:8:ILE:HD11   | 46:BX:43:VAL:HA   | 1.95                     | 0.49              |
| 46:BX:64:LYS:HZ2   | 46:BX:73:ARG:NH2  | 2.08                     | 0.49              |
| 47:BY:50:ARG:HG3   | 47:BY:58:GLY:CA   | 2.39                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 47:BY:87:LYS:NZ   | 47:BY:89:PHE:HE1 | 2.11                     | 0.49              |
| 1:CA:218:C:O2'    | 1:CA:219:C:C6    | 2.64                     | 0.49              |
| 1:CA:438:G:H22    | 1:CA:494:U:H3'   | 1.77                     | 0.49              |
| 1:CA:538:G:O3'    | 12:CL:111:LYS:CE | 2.61                     | 0.49              |
| 1:CA:964:A:H2     | 1:CA:969:A:O2'   | 1.95                     | 0.49              |
| 1:CA:982:U:C6     | 1:CA:983:A:N6    | 2.81                     | 0.49              |
| 2:CB:80:ILE:HG12  | 2:CB:80:ILE:O    | 2.11                     | 0.49              |
| 1:CA:1057:G:H5''  | 3:CC:154:SER:CB  | 2.41                     | 0.49              |
| 5:CE:10:MET:CA    | 5:CE:32:VAL:HG13 | 2.36                     | 0.49              |
| 5:CE:34:VAL:O     | 5:CE:41:VAL:HA   | 2.12                     | 0.49              |
| 5:CE:28:PHE:HE1   | 5:CE:49:PRO:O    | 1.95                     | 0.49              |
| 6:CF:16:GLN:H     | 6:CF:16:GLN:CD   | 2.13                     | 0.49              |
| 7:CG:47:CYS:SG    | 7:CG:58:PRO:HB3  | 2.52                     | 0.49              |
| 9:CI:97:LYS:HB3   | 9:CI:98:PRO:CD   | 2.38                     | 0.49              |
| 15:CO:28:GLN:O    | 15:CO:32:LEU:HG  | 2.13                     | 0.49              |
| 17:CQ:10:VAL:HA   | 17:CQ:20:THR:O   | 2.12                     | 0.49              |
| 1:CA:1320:C:O2    | 19:CS:36:ARG:NH2 | 2.46                     | 0.49              |
| 21:CU:12:LYS:HD2  | 21:CU:17:THR:OG1 | 2.12                     | 0.49              |
| 1:CA:1327:C:OP1   | 21:CU:20:LYS:N   | 2.44                     | 0.49              |
| 50:D1:46:LEU:HD22 | 50:D1:46:LEU:H   | 1.77                     | 0.49              |
| 51:D2:56:GLN:O    | 51:D2:58:ALA:N   | 2.45                     | 0.49              |
| 53:D4:40:ILE:HG22 | 53:D4:41:ILE:N   | 2.27                     | 0.49              |
| 27:DA:1022:G:OP2  | 36:DN:69:GLN:OE1 | 2.30                     | 0.49              |
| 27:DA:1419:A:C8   | 27:DA:1421:G:C6  | 3.01                     | 0.49              |
| 27:DA:1630:G:O2'  | 27:DA:1631:C:H5' | 2.12                     | 0.49              |
| 27:DA:1776:G:O2'  | 27:DA:1777:U:H5' | 2.13                     | 0.49              |
| 27:DA:1946:U:H2'  | 27:DA:1947:C:C6  | 2.40                     | 0.49              |
| 27:DA:2008:C:O2'  | 27:DA:2009:G:H5' | 2.12                     | 0.49              |
| 27:DA:2266:A:H1'  | 27:DA:2272:U:C4  | 2.48                     | 0.49              |
| 27:DA:2266:A:H1'  | 27:DA:2272:U:O4  | 2.12                     | 0.49              |
| 27:DA:2291:U:H2'  | 27:DA:2292:C:C5  | 2.46                     | 0.49              |
| 27:DA:2296:U:O2   | 27:DA:2333:A:N3  | 2.45                     | 0.49              |
| 27:DA:2397:G:H2'  | 27:DA:2398:U:H6  | 1.78                     | 0.49              |
| 27:DA:2726:U:O4'  | 27:DA:2726:U:O2  | 2.31                     | 0.49              |
| 27:DA:2779:U:OP1  | 27:DA:2779:U:H3' | 2.12                     | 0.49              |
| 27:DA:2881:C:O2'  | 27:DA:2882:A:H5' | 2.12                     | 0.49              |
| 27:DA:552:G:C1'   | 27:DA:1220:A:C2  | 2.95                     | 0.49              |
| 27:DA:663:G:H2'   | 27:DA:664:C:H6   | 1.76                     | 0.49              |
| 27:DA:947:G:O6    | 27:DA:970:C:N4   | 2.40                     | 0.49              |
| 30:DD:24:ILE:O    | 30:DD:26:LYS:CE  | 2.60                     | 0.49              |
| 30:DD:30:GLU:OE2  | 30:DD:83:GLU:OE1 | 2.29                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DE:59:VAL:CG2  | 31:DE:60:ASN:N    | 2.69                     | 0.49              |
| 31:DE:6:GLY:HA2   | 31:DE:51:PHE:CE2  | 2.47                     | 0.49              |
| 36:DN:35:ARG:HB3  | 36:DN:42:TRP:CH2  | 2.46                     | 0.49              |
| 36:DN:56:ASN:O    | 36:DN:57:ALA:O    | 2.30                     | 0.49              |
| 37:DO:7:TYR:CD1   | 37:DO:20:MET:HE3  | 2.47                     | 0.49              |
| 38:DP:84:ASN:ND2  | 38:DP:116:GLY:HA3 | 2.26                     | 0.49              |
| 38:DP:130:PHE:N   | 38:DP:130:PHE:HD2 | 2.09                     | 0.49              |
| 38:DP:146:VAL:CG2 | 38:DP:147:LEU:H   | 2.14                     | 0.49              |
| 42:DT:23:ARG:HE   | 42:DT:120:ARG:NH1 | 2.08                     | 0.49              |
| 31:DE:9:VAL:CG2   | 42:DT:8:LYS:HD2   | 2.42                     | 0.49              |
| 48:DZ:52:ILE:CD1  | 48:DZ:52:ILE:H    | 2.14                     | 0.49              |
| 48:DZ:18:ARG:CB   | 48:DZ:81:ARG:HH22 | 2.17                     | 0.49              |
| 1:AA:1158:C:O2'   | 1:AA:1159:U:H4'   | 2.12                     | 0.49              |
| 1:AA:960:U:O2'    | 1:AA:1223:C:C5'   | 2.58                     | 0.49              |
| 1:AA:1278:U:H5'   | 1:AA:1279:A:C8    | 2.47                     | 0.49              |
| 1:AA:1524:C:H2'   | 1:AA:1525:G:O4'   | 2.13                     | 0.49              |
| 1:AA:309:G:H2'    | 1:AA:310:G:H8     | 1.78                     | 0.49              |
| 2:AB:95:GLN:NE2   | 2:AB:147:LYS:HE2  | 2.26                     | 0.49              |
| 3:AC:191:THR:HB   | 3:AC:193:TYR:CE2  | 2.48                     | 0.49              |
| 8:AH:100:ILE:HG22 | 8:AH:125:ARG:HH22 | 1.77                     | 0.49              |
| 8:AH:49:GLU:O     | 8:AH:51:VAL:HG13  | 2.12                     | 0.49              |
| 9:AI:118:LYS:HD3  | 9:AI:121:ARG:CB   | 2.43                     | 0.49              |
| 12:AL:25:LYS:C    | 12:AL:27:ALA:N    | 2.61                     | 0.49              |
| 1:AA:1330:U:O3'   | 13:AM:23:TYR:HE2  | 1.94                     | 0.49              |
| 1:AA:136:C:H1'    | 16:AP:1:MET:HG3   | 1.95                     | 0.49              |
| 19:AS:10:PHE:HZ   | 19:AS:70:LYS:NZ   | 1.92                     | 0.49              |
| 23:AW:72:G:H4'    | 23:AW:72:G:OP1    | 2.12                     | 0.49              |
| 24:AX:48:C:N4     | 24:AX:59:A:C8     | 2.80                     | 0.49              |
| 25:AY:26:C:O2'    | 25:AY:27:C:H5'    | 2.12                     | 0.49              |
| 52:B3:31:LEU:O    | 52:B3:32:GLN:HB2  | 2.12                     | 0.49              |
| 55:B6:11:LEU:CG   | 55:B6:51:GLU:HG2  | 2.43                     | 0.49              |
| 27:BA:1165:U:H2'  | 27:BA:1166:C:C6   | 2.47                     | 0.49              |
| 27:BA:1296:G:HO2' | 27:BA:1297:C:H5'  | 1.75                     | 0.49              |
| 27:BA:1818:U:HO2' | 30:BD:155:LEU:HA  | 1.77                     | 0.49              |
| 27:BA:2150:U:H2'  | 27:BA:2151:G:C8   | 2.47                     | 0.49              |
| 27:BA:2378:A:C5   | 27:BA:2379:G:H1'  | 2.47                     | 0.49              |
| 27:BA:2565:A:H2'  | 27:BA:2566:A:O4'  | 2.12                     | 0.49              |
| 27:BA:265:A:H1'   | 27:BA:266:G:O4'   | 2.12                     | 0.49              |
| 27:BA:2670:A:O2'  | 27:BA:2671:A:H5'  | 2.12                     | 0.49              |
| 27:BA:2724:C:OP1  | 31:BE:118:LYS:HE3 | 2.12                     | 0.49              |
| 30:BD:65:ILE:CG1  | 30:BD:105:ILE:HA  | 2.42                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BD:146:GLU:HG2 | 30:BD:152:GLY:C    | 2.32                     | 0.49              |
| 31:BE:170:LEU:HB3 | 31:BE:184:VAL:CG1  | 2.42                     | 0.49              |
| 31:BE:82:ARG:O    | 31:BE:83:ASP:C     | 2.50                     | 0.49              |
| 33:BG:43:LEU:HB2  | 33:BG:88:ILE:HD13  | 1.94                     | 0.49              |
| 35:BI:82:ARG:O    | 35:BI:88:ILE:HG23  | 2.13                     | 0.49              |
| 37:BO:69:ILE:HG13 | 37:BO:77:ILE:HG22  | 1.93                     | 0.49              |
| 38:BP:10:PRO:O    | 38:BP:11:GLY:C     | 2.48                     | 0.49              |
| 38:BP:111:ARG:NH1 | 38:BP:149:GLU:HG3  | 2.27                     | 0.49              |
| 39:BQ:2:LEU:HB3   | 39:BQ:44:ALA:HB1   | 1.94                     | 0.49              |
| 42:BT:67:SER:O    | 42:BT:68:TYR:HB2   | 2.10                     | 0.49              |
| 47:BY:51:VAL:O    | 47:BY:51:VAL:HG12  | 2.11                     | 0.49              |
| 48:BZ:25:GLY:HA2  | 48:BZ:84:HIS:CD2   | 2.47                     | 0.49              |
| 1:CA:217:C:HO2'   | 1:CA:218:C:H6      | 1.53                     | 0.49              |
| 1:CA:244:U:C6     | 1:CA:894:G:N2      | 2.80                     | 0.49              |
| 1:CA:273:A:C2'    | 1:CA:274:A:H5'     | 2.43                     | 0.49              |
| 1:CA:398:C:H2'    | 1:CA:399:G:C8      | 2.47                     | 0.49              |
| 1:CA:443:C:H2'    | 1:CA:444:C:C6      | 2.47                     | 0.49              |
| 1:CA:491:G:C6     | 1:CA:492:G:C5      | 3.00                     | 0.49              |
| 1:CA:405:U:H5''   | 1:CA:495:A:H2      | 1.76                     | 0.49              |
| 1:CA:509:A:C2     | 1:CA:510:A:C2      | 3.00                     | 0.49              |
| 1:CA:591:U:C2     | 1:CA:649:G:N2      | 2.80                     | 0.49              |
| 1:CA:762:C:H6     | 1:CA:762:C:O5'     | 1.94                     | 0.49              |
| 1:CA:979:C:C5     | 1:CA:980:C:C6      | 3.01                     | 0.49              |
| 3:CC:3:ASN:O      | 3:CC:4:LYS:CB      | 2.57                     | 0.49              |
| 5:CE:59:GLY:O     | 5:CE:62:ALA:HB3    | 2.12                     | 0.49              |
| 10:CJ:85:LEU:C    | 10:CJ:87:THR:N     | 2.65                     | 0.49              |
| 12:CL:98:VAL:CG1  | 12:CL:101:VAL:HG21 | 2.42                     | 0.49              |
| 13:CM:25:ILE:N    | 13:CM:25:ILE:CD1   | 2.75                     | 0.49              |
| 13:CM:83:ASP:HB2  | 19:CS:66:MET:CE    | 2.42                     | 0.49              |
| 14:CN:24:CYS:HB3  | 14:CN:29:ARG:HB3   | 1.94                     | 0.49              |
| 15:CO:70:LEU:HD11 | 15:CO:77:ARG:HE    | 1.77                     | 0.49              |
| 15:CO:78:TYR:O    | 15:CO:82:ILE:HG22  | 2.12                     | 0.49              |
| 18:CR:51:LEU:HB2  | 18:CR:56:THR:HG22  | 1.94                     | 0.49              |
| 25:CY:25:A:C2'    | 25:CY:26:C:H5'     | 2.42                     | 0.49              |
| 50:D1:51:VAL:HG22 | 50:D1:52:ARG:N     | 2.27                     | 0.49              |
| 27:DA:124:G:C5    | 56:D7:19:ARG:NH2   | 2.80                     | 0.49              |
| 27:DA:1133:U:O2'  | 27:DA:1135:C:H5''  | 2.12                     | 0.49              |
| 27:DA:1248:G:H3'  | 27:DA:1249:U:C5'   | 2.40                     | 0.49              |
| 27:DA:1306:C:O2   | 27:DA:1623:G:C6    | 2.65                     | 0.49              |
| 27:DA:1348:G:C3'  | 27:DA:1349:A:H5''  | 2.41                     | 0.49              |
| 27:DA:1569:A:O2'  | 27:DA:1570:A:H5'   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:1697:G:H3'  | 27:DA:1698:A:C5'   | 2.42                     | 0.49              |
| 27:DA:1754:C:N4   | 27:DA:1755:A:N6    | 2.60                     | 0.49              |
| 27:DA:1865:G:N2   | 27:DA:1878:G:C5    | 2.80                     | 0.49              |
| 27:DA:1794:U:H1'  | 27:DA:1900:A:N3    | 2.27                     | 0.49              |
| 27:DA:647:G:N2    | 27:DA:2350:C:H4'   | 2.14                     | 0.49              |
| 27:DA:240:G:C6    | 27:DA:241:A:N6     | 2.80                     | 0.49              |
| 27:DA:2425:A:H4'  | 27:DA:2426:A:O5'   | 2.13                     | 0.49              |
| 27:DA:2731:G:C6   | 27:DA:2732:G:O6    | 2.65                     | 0.49              |
| 27:DA:2804:C:O2'  | 27:DA:2805:G:H5'   | 2.13                     | 0.49              |
| 27:DA:297:C:O2'   | 27:DA:298:G:H5'    | 2.12                     | 0.49              |
| 27:DA:372:G:H22   | 27:DA:400:G:H2'    | 1.76                     | 0.49              |
| 27:DA:448:U:H3'   | 27:DA:449:A:H5'    | 1.95                     | 0.49              |
| 30:DD:118:VAL:CG2 | 30:DD:119:ALA:N    | 2.60                     | 0.49              |
| 30:DD:28:GLU:H    | 30:DD:29:PRO:HD2   | 1.77                     | 0.49              |
| 30:DD:34:VAL:O    | 30:DD:34:VAL:HG13  | 2.11                     | 0.49              |
| 33:DG:104:GLU:HG2 | 53:D4:50:THR:HG21  | 1.93                     | 0.49              |
| 33:DG:33:ARG:CZ   | 33:DG:162:THR:HG21 | 2.43                     | 0.49              |
| 34:DH:150:ALA:C   | 34:DH:152:ARG:N    | 2.66                     | 0.49              |
| 27:DA:1137:G:N2   | 36:DN:106:MET:HG2  | 2.26                     | 0.49              |
| 36:DN:48:MET:H    | 36:DN:48:MET:HE2   | 1.76                     | 0.49              |
| 36:DN:66:LYS:O    | 36:DN:70:LYS:HB2   | 2.13                     | 0.49              |
| 38:DP:29:LYS:N    | 38:DP:29:LYS:HD2   | 2.28                     | 0.49              |
| 40:DR:34:ILE:O    | 40:DR:113:LEU:HD12 | 2.12                     | 0.49              |
| 40:DR:62:ALA:O    | 40:DR:66:VAL:HG23  | 2.12                     | 0.49              |
| 41:DS:96:GLY:O    | 41:DS:98:VAL:N     | 2.46                     | 0.49              |
| 45:DW:50:VAL:HG21 | 45:DW:105:VAL:HG23 | 1.93                     | 0.49              |
| 46:DX:36:LYS:HE2  | 46:DX:56:THR:H     | 1.78                     | 0.49              |
| 47:DY:54:LYS:O    | 47:DY:55:TYR:CD1   | 2.66                     | 0.49              |
| 47:DY:9:LYS:O     | 47:DY:28:LYS:NZ    | 2.41                     | 0.49              |
| 48:DZ:158:PRO:C   | 48:DZ:160:VAL:H    | 2.16                     | 0.49              |
| 48:DZ:60:LEU:N    | 48:DZ:60:LEU:CD2   | 2.76                     | 0.49              |
| 1:AA:1265:G:C3'   | 1:AA:1265:G:C8     | 2.96                     | 0.49              |
| 1:AA:1271:G:H2'   | 1:AA:1272:G:H8     | 1.76                     | 0.49              |
| 1:AA:802:A:H2'    | 1:AA:803:G:O4'     | 2.13                     | 0.49              |
| 1:AA:939:G:C6     | 1:AA:940:C:N4      | 2.80                     | 0.49              |
| 2:AB:114:ARG:CA   | 2:AB:117:GLU:HB2   | 2.41                     | 0.49              |
| 2:AB:70:PHE:CE2   | 2:AB:163:PHE:HD1   | 2.31                     | 0.49              |
| 2:AB:166:ASP:OD1  | 2:AB:169:LYS:HB2   | 2.11                     | 0.49              |
| 5:AE:107:ARG:HG3  | 5:AE:111:GLU:HG3   | 1.93                     | 0.49              |
| 5:AE:81:GLU:HA    | 5:AE:89:ILE:O      | 2.12                     | 0.49              |
| 8:AH:4:ASP:OD2    | 8:AH:85:ARG:NH1    | 2.39                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AK:80:VAL:HG22  | 11:AK:103:LEU:HD12 | 1.94                     | 0.49              |
| 12:AL:119:THR:CG2  | 12:AL:120:LYS:H    | 2.26                     | 0.49              |
| 12:AL:24:LEU:O     | 12:AL:26:GLY:N     | 2.46                     | 0.49              |
| 13:AM:105:THR:O    | 13:AM:106:ASN:HB2  | 2.12                     | 0.49              |
| 13:AM:8:GLU:OE1    | 13:AM:22:ILE:HG23  | 2.12                     | 0.49              |
| 17:AQ:79:SER:O     | 17:AQ:80:GLY:C     | 2.50                     | 0.49              |
| 18:AR:37:VAL:CG1   | 18:AR:78:LEU:HB3   | 2.43                     | 0.49              |
| 27:BA:2336:A:H61   | 49:B0:43:THR:HG21  | 1.77                     | 0.49              |
| 51:B2:7:ARG:CG     | 51:B2:7:ARG:HH11   | 2.26                     | 0.49              |
| 54:B5:52:TYR:CD1   | 54:B5:52:TYR:O     | 2.65                     | 0.49              |
| 56:B7:31:LEU:HD22  | 56:B7:42:LEU:HD13  | 1.94                     | 0.49              |
| 57:B8:42:ARG:C     | 57:B8:44:LYS:H     | 2.15                     | 0.49              |
| 27:BA:1049:C:O2'   | 27:BA:1050:A:C8    | 2.61                     | 0.49              |
| 27:BA:1128:A:H3'   | 27:BA:1128:A:OP2   | 2.12                     | 0.49              |
| 27:BA:1409:C:H2'   | 27:BA:1410:G:C8    | 2.48                     | 0.49              |
| 27:BA:195:A:H61    | 27:BA:198:C:H3'    | 1.77                     | 0.49              |
| 27:BA:2173:A:H2'   | 27:BA:2174:C:C6    | 2.48                     | 0.49              |
| 27:BA:2323:G:H2'   | 27:BA:2324:C:O4'   | 2.12                     | 0.49              |
| 27:BA:2331:G:O4'   | 49:B0:42:GLY:HA3   | 2.13                     | 0.49              |
| 27:BA:2849:U:H1'   | 27:BA:2866:U:H6    | 1.77                     | 0.49              |
| 27:BA:2875:C:C4    | 27:BA:2876:G:N7    | 2.80                     | 0.49              |
| 27:BA:538:G:C2     | 27:BA:556:G:C6     | 3.01                     | 0.49              |
| 30:BD:28:GLU:HB2   | 30:BD:29:PRO:CD    | 2.42                     | 0.49              |
| 30:BD:31:LYS:CE    | 30:BD:94:LEU:HD11  | 2.43                     | 0.49              |
| 31:BE:116:VAL:HG21 | 31:BE:122:PHE:CE2  | 2.47                     | 0.49              |
| 32:BF:132:VAL:CG1  | 32:BF:133:ASN:N    | 2.67                     | 0.49              |
| 32:BF:19:GLU:N     | 32:BF:19:GLU:OE2   | 2.46                     | 0.49              |
| 33:BG:181:ARG:HG2  | 33:BG:181:ARG:O    | 2.13                     | 0.49              |
| 36:BN:133:GLN:C    | 36:BN:134:ARG:CG   | 2.81                     | 0.49              |
| 41:BS:59:LYS:HE3   | 41:BS:68:GLN:OE1   | 2.13                     | 0.49              |
| 42:BT:78:LEU:HB3   | 42:BT:79:HIS:CE1   | 2.47                     | 0.49              |
| 43:BU:25:TRP:HD1   | 43:BU:26:GLY:N     | 2.07                     | 0.49              |
| 1:CA:182:U:OP2     | 1:CA:183:G:N7      | 2.46                     | 0.49              |
| 1:CA:199:G:O2'     | 1:CA:200:G:O5'     | 2.30                     | 0.49              |
| 1:CA:25:C:H5'      | 1:CA:524:G:O2'     | 2.13                     | 0.49              |
| 1:CA:28:G:C2       | 1:CA:556:C:N3      | 2.81                     | 0.49              |
| 1:CA:653:A:H1'     | 8:CH:56:LYS:HZ3    | 1.78                     | 0.49              |
| 1:CA:619:U:N3      | 4:CD:135:LEU:HD21  | 2.27                     | 0.49              |
| 4:CD:79:PHE:HA     | 4:CD:93:PHE:CD2    | 2.47                     | 0.49              |
| 11:CK:96:ARG:HA    | 11:CK:99:GLN:CG    | 2.41                     | 0.49              |
| 1:CA:1321:C:H4'    | 13:CM:87:TYR:CZ    | 2.46                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:CN:34:TYR:N    | 14:CN:34:TYR:HD1   | 2.10                     | 0.49              |
| 20:CT:50:GLU:HG3  | 20:CT:51:GLU:N     | 2.28                     | 0.49              |
| 1:CA:1325:C:H4'   | 21:CU:17:THR:HG21  | 1.95                     | 0.49              |
| 7:CG:86:GLN:NE2   | 25:CY:30:A:H2      | 2.09                     | 0.49              |
| 27:DA:2355:C:H1'  | 49:D0:36:ILE:HD11  | 1.93                     | 0.49              |
| 56:D7:34:ARG:HH11 | 56:D7:42:LEU:HA    | 1.75                     | 0.49              |
| 27:DA:1494:A:N3   | 27:DA:1494:A:H2'   | 2.27                     | 0.49              |
| 27:DA:1578:U:H2'  | 27:DA:1579:A:C5'   | 2.43                     | 0.49              |
| 27:DA:1659:U:C4   | 27:DA:1660:C:C5    | 3.01                     | 0.49              |
| 27:DA:174:C:O2    | 27:DA:174:C:H2'    | 2.11                     | 0.49              |
| 27:DA:1991:U:C2'  | 27:DA:1992:G:C5'   | 2.90                     | 0.49              |
| 27:DA:2126:A:N1   | 27:DA:2163:C:H4'   | 2.27                     | 0.49              |
| 27:DA:2396:G:H4'  | 50:D1:30:VAL:H     | 1.78                     | 0.49              |
| 27:DA:2422:A:H4'  | 27:DA:2423:U:OP1   | 2.12                     | 0.49              |
| 27:DA:2067:G:N2   | 27:DA:2444:G:C4    | 2.81                     | 0.49              |
| 27:DA:2542:A:O2'  | 27:DA:2543:G:C8    | 2.61                     | 0.49              |
| 27:DA:2656:U:H2'  | 27:DA:2657:A:H8    | 1.77                     | 0.49              |
| 27:DA:2830:G:O2'  | 27:DA:2883:A:N1    | 2.39                     | 0.49              |
| 27:DA:495:G:H1'   | 45:DW:57:ASN:ND2   | 2.26                     | 0.49              |
| 27:DA:579:G:C2    | 27:DA:1262:A:C5    | 3.01                     | 0.49              |
| 27:DA:588:U:O2'   | 27:DA:589:C:C5'    | 2.60                     | 0.49              |
| 27:DA:629:G:C6    | 27:DA:630:G:C6     | 3.00                     | 0.49              |
| 27:DA:695:G:C2    | 27:DA:768:G:C5     | 3.01                     | 0.49              |
| 28:DB:45:A:H2'    | 28:DB:46:A:H5'     | 1.93                     | 0.49              |
| 28:DB:88:C:H2'    | 28:DB:89:G:H8      | 1.76                     | 0.49              |
| 29:DC:107:TRP:O   | 29:DC:108:MET:CB   | 2.61                     | 0.49              |
| 30:DD:124:PRO:HG2 | 30:DD:129:ASN:HD21 | 1.76                     | 0.49              |
| 30:DD:108:PRO:HG3 | 30:DD:143:HIS:NE2  | 2.27                     | 0.49              |
| 30:DD:183:ARG:HG2 | 30:DD:183:ARG:HH11 | 1.78                     | 0.49              |
| 27:DA:1569:A:C1'  | 30:DD:38:LYS:HZ3   | 2.25                     | 0.49              |
| 30:DD:90:ALA:CB   | 30:DD:106:ILE:HG13 | 2.42                     | 0.49              |
| 34:DH:18:GLU:HB2  | 34:DH:25:LYS:HG2   | 1.93                     | 0.49              |
| 34:DH:41:MET:HG2  | 34:DH:52:VAL:HG13  | 1.94                     | 0.49              |
| 36:DN:125:GLY:CA  | 36:DN:126:PRO:O    | 2.58                     | 0.49              |
| 36:DN:22:THR:HG22 | 36:DN:23:LEU:HD23  | 1.94                     | 0.49              |
| 36:DN:87:LEU:HD21 | 36:DN:98:VAL:HG11  | 1.94                     | 0.49              |
| 37:DO:7:TYR:HE1   | 37:DO:20:MET:HE3   | 1.75                     | 0.49              |
| 38:DP:107:LYS:HG3 | 38:DP:107:LYS:O    | 2.12                     | 0.49              |
| 27:DA:627:A:N7    | 38:DP:84:ASN:ND2   | 2.60                     | 0.49              |
| 40:DR:104:ARG:HG3 | 40:DR:111:LEU:HD21 | 1.94                     | 0.49              |
| 41:DS:58:LEU:HD21 | 41:DS:69:VAL:HB    | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DS:78:LEU:HD21 | 41:DS:103:GLU:HB3 | 1.95                     | 0.49              |
| 41:DS:97:ARG:HH12 | 41:DS:99:LYS:CD   | 2.25                     | 0.49              |
| 42:DT:16:ARG:HH12 | 42:DT:19:LEU:HD21 | 1.77                     | 0.49              |
| 45:DW:62:HIS:O    | 45:DW:63:ASP:C    | 2.49                     | 0.49              |
| 45:DW:86:LEU:HD23 | 45:DW:96:ILE:HB   | 1.95                     | 0.49              |
| 47:DY:10:GLY:O    | 47:DY:27:VAL:HG22 | 2.13                     | 0.49              |
| 1:AA:865:A:H5'    | 1:AA:1078:U:O4    | 2.13                     | 0.49              |
| 1:AA:1164:G:H2'   | 1:AA:1165:C:H6    | 1.76                     | 0.49              |
| 1:AA:1229:A:H2'   | 1:AA:1230:C:H6    | 1.78                     | 0.49              |
| 1:AA:444:C:N4     | 1:AA:490:G:H1     | 2.11                     | 0.49              |
| 1:AA:514:C:O2'    | 1:AA:515:G:H5'    | 2.12                     | 0.49              |
| 1:AA:514:C:O2     | 1:AA:538:G:N2     | 2.46                     | 0.49              |
| 2:AB:75:LYS:HA    | 2:AB:78:GLN:HB2   | 1.94                     | 0.49              |
| 3:AC:150:LYS:HE3  | 3:AC:167:TRP:CD1  | 2.47                     | 0.49              |
| 4:AD:76:ARG:O     | 4:AD:77:ASN:C     | 2.51                     | 0.49              |
| 1:AA:1373:G:H5''  | 7:AG:36:LYS:HB2   | 1.94                     | 0.49              |
| 10:AJ:32:ALA:H    | 10:AJ:76:ASN:CB   | 2.25                     | 0.49              |
| 12:AL:87:VAL:HG12 | 12:AL:90:LEU:H    | 1.77                     | 0.49              |
| 51:B2:25:VAL:O    | 51:B2:26:ARG:C    | 2.50                     | 0.49              |
| 53:B4:42:CYS:HA   | 53:B4:59:VAL:HB   | 1.95                     | 0.49              |
| 57:B8:10:ALA:O    | 57:B8:13:ARG:N    | 2.36                     | 0.49              |
| 27:BA:1050:A:O2'  | 27:BA:1051:G:H8   | 1.93                     | 0.49              |
| 27:BA:1458:C:H5'  | 27:BA:1459:G:C8   | 2.48                     | 0.49              |
| 27:BA:2056:G:H1   | 54:B5:4:HIS:HD2   | 1.61                     | 0.49              |
| 27:BA:2163:C:OP2  | 27:BA:2164:C:H5   | 1.95                     | 0.49              |
| 27:BA:2321:G:C2'  | 27:BA:2321:G:N3   | 2.65                     | 0.49              |
| 27:BA:2889:C:O2   | 27:BA:2889:C:H2'  | 2.12                     | 0.49              |
| 27:BA:510:C:O5'   | 27:BA:510:C:H6    | 1.94                     | 0.49              |
| 27:BA:707:G:H5'   | 27:BA:708:C:P     | 2.53                     | 0.49              |
| 27:BA:817:C:O2'   | 27:BA:839:U:OP1   | 2.30                     | 0.49              |
| 27:BA:875:G:C2'   | 27:BA:876:C:H5'   | 2.43                     | 0.49              |
| 27:BA:894:C:H2'   | 27:BA:895:U:C6    | 2.46                     | 0.49              |
| 27:BA:92:A:H1'    | 27:BA:93:G:C8     | 2.45                     | 0.49              |
| 32:BF:127:GLU:HG2 | 32:BF:196:LEU:CD1 | 2.42                     | 0.49              |
| 33:BG:55:LYS:NZ   | 33:BG:148:MET:HE3 | 2.28                     | 0.49              |
| 34:BH:99:VAL:O    | 34:BH:102:ALA:HB3 | 2.12                     | 0.49              |
| 34:BH:156:ALA:H   | 34:BH:158:HIS:H   | 1.60                     | 0.49              |
| 34:BH:47:GLU:C    | 34:BH:49:VAL:H    | 2.15                     | 0.49              |
| 37:BO:6:THR:HG22  | 37:BO:7:TYR:N     | 2.28                     | 0.49              |
| 38:BP:107:LYS:C   | 38:BP:109:GLY:N   | 2.58                     | 0.49              |
| 38:BP:64:LYS:O    | 38:BP:65:ARG:C    | 2.48                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:BT:31:SER:HB2   | 42:BT:32:TYR:CD2  | 2.48                     | 0.49              |
| 46:BX:3:THR:O      | 46:BX:4:ALA:HB3   | 2.12                     | 0.49              |
| 27:BA:64:A:C1'     | 46:BX:66:LEU:HB2  | 2.38                     | 0.49              |
| 47:BY:77:PRO:O     | 47:BY:99:CYS:SG   | 2.71                     | 0.49              |
| 48:BZ:156:LEU:HB3  | 48:BZ:160:VAL:CG1 | 2.41                     | 0.49              |
| 48:BZ:43:PHE:CE2   | 48:BZ:85:VAL:HG11 | 2.48                     | 0.49              |
| 1:CA:1138:G:N2     | 1:CA:1140:C:C4    | 2.81                     | 0.49              |
| 1:CA:1254:C:N4     | 10:CJ:43:ARG:HH12 | 2.11                     | 0.49              |
| 1:CA:1343:G:C5     | 1:CA:1344:C:C4    | 3.01                     | 0.49              |
| 1:CA:30:U:H4'      | 1:CA:31:G:OP1     | 2.10                     | 0.49              |
| 1:CA:346:G:H5'     | 42:DT:41:ARG:CZ   | 2.41                     | 0.49              |
| 1:CA:668:G:H2'     | 1:CA:669:U:C6     | 2.47                     | 0.49              |
| 1:CA:827:U:H2'     | 1:CA:870:U:O4     | 2.13                     | 0.49              |
| 3:CC:11:ARG:O      | 3:CC:12:LEU:C     | 2.50                     | 0.49              |
| 8:CH:28:ALA:HA     | 8:CH:59:LEU:CG    | 2.42                     | 0.49              |
| 9:CI:97:LYS:HZ3    | 9:CI:97:LYS:HB2   | 1.78                     | 0.49              |
| 13:CM:88:ARG:HA    | 13:CM:98:VAL:HG11 | 1.91                     | 0.49              |
| 1:CA:1060:C:C5'    | 14:CN:45:ARG:NH2  | 2.72                     | 0.49              |
| 15:CO:6:GLU:O      | 15:CO:9:GLN:N     | 2.46                     | 0.49              |
| 1:CA:1220:G:O3'    | 19:CS:36:ARG:HD3  | 2.12                     | 0.49              |
| 24:CX:47:U:C2      | 24:CX:50:U:OP1    | 2.66                     | 0.49              |
| 50:D1:71:TYR:HD1   | 50:D1:71:TYR:H    | 1.60                     | 0.49              |
| 51:D2:4:SER:HA     | 51:D2:7:ARG:HG2   | 1.94                     | 0.49              |
| 27:DA:1152:C:H2'   | 27:DA:1153:C:C6   | 2.47                     | 0.49              |
| 27:DA:1170:G:H8    | 27:DA:1170:G:OP2  | 1.96                     | 0.49              |
| 27:DA:1174:A:OP1   | 27:DA:1175:U:H5'' | 2.12                     | 0.49              |
| 27:DA:1629:U:O5'   | 27:DA:1629:U:H6   | 1.96                     | 0.49              |
| 27:DA:1885:A:C8    | 27:DA:1886:C:C6   | 3.00                     | 0.49              |
| 27:DA:1934:C:H2'   | 27:DA:1935:G:C8   | 2.47                     | 0.49              |
| 27:DA:1982:C:O2'   | 27:DA:1983:C:H5'  | 2.12                     | 0.49              |
| 27:DA:1987:G:H5'   | 27:DA:1988:C:OP2  | 2.12                     | 0.49              |
| 27:DA:2292:C:H42   | 27:DA:2340:G:H1   | 1.60                     | 0.49              |
| 27:DA:271(C):C:H2' | 27:DA:271(D):G:C8 | 2.48                     | 0.49              |
| 27:DA:7:G:H2'      | 27:DA:8:A:C8      | 2.48                     | 0.49              |
| 27:DA:951:C:O2'    | 27:DA:952:G:H5'   | 2.12                     | 0.49              |
| 30:DD:40:THR:HG22  | 30:DD:41:GLY:O    | 2.13                     | 0.49              |
| 31:DE:143:ASN:HB2  | 31:DE:146:THR:O   | 2.12                     | 0.49              |
| 32:DF:132:VAL:HG13 | 32:DF:133:ASN:H   | 1.77                     | 0.49              |
| 32:DF:32:LEU:C     | 32:DF:32:LEU:HD23 | 2.33                     | 0.49              |
| 32:DF:3:GLU:CD     | 32:DF:3:GLU:H     | 2.14                     | 0.49              |
| 33:DG:4:ASP:HA     | 33:DG:8:LYS:HD2   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DG:50:ALA:O    | 33:DG:52:ILE:N     | 2.45                     | 0.49              |
| 34:DH:20:ALA:HB1  | 34:DH:21:PRO:CD    | 2.42                     | 0.49              |
| 35:DI:75:LEU:HD21 | 35:DI:105:HIS:ND1  | 2.27                     | 0.49              |
| 37:DO:35:VAL:HG22 | 37:DO:65:THR:HG23  | 1.95                     | 0.49              |
| 42:DT:106:SER:HB2 | 42:DT:110:ILE:HD12 | 1.95                     | 0.49              |
| 45:DW:25:ARG:NH1  | 45:DW:25:ARG:CB    | 2.76                     | 0.49              |
| 47:DY:13:VAL:HG23 | 47:DY:14:LEU:N     | 2.28                     | 0.49              |
| 48:DZ:150:HIS:HA  | 48:DZ:169:THR:HA   | 1.94                     | 0.49              |
| 1:AA:1038:C:H2'   | 1:AA:1039:C:C5     | 2.47                     | 0.49              |
| 1:AA:1142:G:H3'   | 1:AA:1143:G:H8     | 1.78                     | 0.49              |
| 1:AA:1293:G:H2'   | 1:AA:1294:G:C8     | 2.47                     | 0.49              |
| 1:AA:1452:C:H4'   | 1:AA:1456:G:N3     | 2.28                     | 0.49              |
| 1:AA:1515:C:H2'   | 1:AA:1515:C:O2     | 2.13                     | 0.49              |
| 1:AA:314:C:O5'    | 1:AA:314:C:H6      | 1.94                     | 0.49              |
| 1:AA:492:G:C5     | 1:AA:493:G:N7      | 2.81                     | 0.49              |
| 1:AA:569:C:H5''   | 1:AA:570:G:OP1     | 2.13                     | 0.49              |
| 1:AA:852:G:O2'    | 1:AA:853:G:H5'     | 2.13                     | 0.49              |
| 2:AB:140:HIS:O    | 2:AB:143:GLU:HB2   | 2.12                     | 0.49              |
| 3:AC:143:GLU:C    | 3:AC:145:GLY:N     | 2.66                     | 0.49              |
| 3:AC:36:ASP:OD2   | 3:AC:57:ILE:HG21   | 2.13                     | 0.49              |
| 5:AE:8:GLU:HB2    | 5:AE:34:VAL:HG22   | 1.95                     | 0.49              |
| 6:AF:44:GLY:C     | 6:AF:59:TYR:HA     | 2.33                     | 0.49              |
| 6:AF:72:VAL:HG13  | 6:AF:73:ASN:N      | 2.28                     | 0.49              |
| 11:AK:32:ILE:CD1  | 11:AK:41:THR:HB    | 2.33                     | 0.49              |
| 13:AM:14:ARG:HE   | 13:AM:42:ALA:HA    | 1.78                     | 0.49              |
| 19:AS:52:TYR:CE1  | 19:AS:56:GLN:HA    | 2.48                     | 0.49              |
| 23:AW:39:C:C2     | 23:AW:40:C:C5      | 3.01                     | 0.49              |
| 55:B6:32:ASN:C    | 55:B6:33:LYS:HG2   | 2.32                     | 0.49              |
| 56:B7:8:ASN:ND2   | 56:B7:11:LYS:N     | 2.53                     | 0.49              |
| 27:BA:1360:A:C6   | 27:BA:1372:U:C5    | 3.01                     | 0.49              |
| 27:BA:1492:G:N2   | 27:BA:1499:C:C2    | 2.81                     | 0.49              |
| 27:BA:1556:C:O2'  | 27:BA:1557:C:C5'   | 2.61                     | 0.49              |
| 27:BA:1591:G:C6   | 27:BA:1592:C:N4    | 2.81                     | 0.49              |
| 27:BA:200:U:C5    | 27:BA:201:C:C6     | 3.01                     | 0.49              |
| 27:BA:2313:C:N4   | 27:BA:2314:C:H41   | 2.11                     | 0.49              |
| 27:BA:2416:C:H2'  | 27:BA:2417:C:H6    | 1.77                     | 0.49              |
| 27:BA:2461:C:O2   | 27:BA:2461:C:H2'   | 2.12                     | 0.49              |
| 27:BA:2468:G:N2   | 27:BA:2481:G:O2'   | 2.45                     | 0.49              |
| 27:BA:2582:G:N2   | 27:BA:2583:G:H1'   | 2.28                     | 0.49              |
| 27:BA:2723:C:H2'  | 27:BA:2724:C:H5'   | 1.94                     | 0.49              |
| 27:BA:274:G:N2    | 27:BA:274:G:OP2    | 2.40                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2777:G:C5'  | 27:BA:2778:A:H5''  | 2.37                     | 0.49              |
| 27:BA:760:G:C2    | 27:BA:761:A:H1'    | 2.48                     | 0.49              |
| 27:BA:878:A:H61   | 27:BA:899:A:H1'    | 1.78                     | 0.49              |
| 27:BA:936:C:O2'   | 27:BA:937:U:H5'    | 2.13                     | 0.49              |
| 27:BA:1569:A:O2'  | 30:BD:38:LYS:HE2   | 2.13                     | 0.49              |
| 33:BG:122:PRO:HG2 | 33:BG:123:ASN:OD1  | 2.13                     | 0.49              |
| 34:BH:85:LYS:HE2  | 34:BH:141:VAL:O    | 2.12                     | 0.49              |
| 34:BH:20:ALA:O    | 34:BH:21:PRO:C     | 2.50                     | 0.49              |
| 34:BH:97:ARG:CG   | 34:BH:98:LEU:H     | 2.11                     | 0.49              |
| 35:BI:12:LEU:CD1  | 35:BI:19:VAL:HG11  | 2.40                     | 0.49              |
| 27:BA:1138:G:N3   | 36:BN:106:MET:HE2  | 2.28                     | 0.49              |
| 36:BN:46:VAL:HG13 | 36:BN:47:ALA:H     | 1.77                     | 0.49              |
| 36:BN:73:THR:HG22 | 36:BN:74:ARG:N     | 2.28                     | 0.49              |
| 37:BO:90:GLN:HB2  | 37:BO:92:GLU:OE2   | 2.12                     | 0.49              |
| 38:BP:80:TYR:CZ   | 38:BP:111:ARG:HD3  | 2.47                     | 0.49              |
| 27:BA:954:G:C5'   | 39:BQ:13:GLN:HG2   | 2.27                     | 0.49              |
| 42:BT:26:ASP:O    | 42:BT:27:THR:O     | 2.30                     | 0.49              |
| 43:BU:106:PHE:O   | 43:BU:110:VAL:HG23 | 2.13                     | 0.49              |
| 44:BV:2:PHE:CD2   | 44:BV:42:GLY:HA2   | 2.45                     | 0.49              |
| 47:BY:48:ALA:HB1  | 47:BY:50:ARG:H     | 1.77                     | 0.49              |
| 48:BZ:26:VAL:HG22 | 48:BZ:27:MET:H     | 1.78                     | 0.49              |
| 1:CA:1015:A:O2'   | 1:CA:1219:U:H5'    | 2.13                     | 0.49              |
| 1:CA:1166:G:N2    | 1:CA:1170:A:OP2    | 2.46                     | 0.49              |
| 1:CA:189(E):U:OP2 | 1:CA:189(E):U:H6   | 1.96                     | 0.49              |
| 1:CA:67:C:OP1     | 1:CA:199:G:H5''    | 2.12                     | 0.49              |
| 1:CA:259:G:H2'    | 1:CA:260:G:O4'     | 2.13                     | 0.49              |
| 1:CA:7:G:O6       | 5:CE:92:LYS:HD2    | 2.13                     | 0.49              |
| 6:CF:97:PHE:HD2   | 18:CR:65:ILE:HD13  | 1.76                     | 0.49              |
| 11:CK:65:ALA:HB1  | 11:CK:98:LEU:HD21  | 1.93                     | 0.49              |
| 20:CT:75:ASN:O    | 20:CT:78:ALA:HB3   | 2.12                     | 0.49              |
| 24:CX:8:U:C5      | 24:CX:15:G:O6      | 2.65                     | 0.49              |
| 24:CX:17:C:C2     | 24:CX:17(B):U:C5   | 3.01                     | 0.49              |
| 49:D0:56:ASP:CG   | 49:D0:58:THR:HG1   | 2.15                     | 0.49              |
| 57:D8:38:GLY:O    | 57:D8:42:ARG:N     | 2.43                     | 0.49              |
| 27:DA:247:G:O6    | 57:D8:8:LYS:HB3    | 2.13                     | 0.49              |
| 27:DA:122:G:O2'   | 27:DA:123:G:H5'    | 2.11                     | 0.49              |
| 27:DA:142:A:H8    | 27:DA:1595:G:N2    | 2.09                     | 0.49              |
| 27:DA:204:A:O2'   | 27:DA:205:G:C4'    | 2.61                     | 0.49              |
| 27:DA:2420:C:OP1  | 57:D8:33:ASN:O     | 2.30                     | 0.49              |
| 27:DA:2645:G:OP2  | 27:DA:2645:G:H8    | 1.96                     | 0.49              |
| 27:DA:2845:G:O2'  | 27:DA:2846:G:H5'   | 2.12                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:324:A:C2     | 27:DA:325:G:C1'    | 2.96                     | 0.49              |
| 27:DA:80:G:H1'     | 27:DA:346:A:C6     | 2.47                     | 0.49              |
| 27:DA:391:G:C2'    | 27:DA:392:C:H5'    | 2.43                     | 0.49              |
| 27:DA:459:U:H5''   | 56:D7:40:TRP:CE3   | 2.48                     | 0.49              |
| 27:DA:491:G:H2'    | 27:DA:492:A:O5'    | 2.13                     | 0.49              |
| 27:DA:588:U:O2'    | 27:DA:589:C:O5'    | 2.31                     | 0.49              |
| 27:DA:745:G:OP2    | 31:DE:133:LYS:HE3  | 2.12                     | 0.49              |
| 28:DB:61:G:O2'     | 28:DB:62:C:H5'     | 2.12                     | 0.49              |
| 29:DC:41:VAL:CG1   | 29:DC:213:TYR:HA   | 2.43                     | 0.49              |
| 30:DD:242:ARG:HG2  | 30:DD:246:PRO:HD3  | 1.94                     | 0.49              |
| 32:DF:119:ARG:HH11 | 32:DF:119:ARG:HG2  | 1.77                     | 0.49              |
| 33:DG:125:PHE:HB3  | 33:DG:130:ASN:O    | 2.13                     | 0.49              |
| 34:DH:86:GLU:CB    | 34:DH:132:ARG:HH11 | 2.26                     | 0.49              |
| 36:DN:46:VAL:CG1   | 36:DN:48:MET:HG3   | 2.42                     | 0.49              |
| 38:DP:100:LEU:HB2  | 38:DP:106:LEU:HD22 | 1.95                     | 0.49              |
| 38:DP:64:LYS:C     | 38:DP:66:GLY:N     | 2.64                     | 0.49              |
| 48:DZ:3:ARG:HB2    | 48:DZ:57:VAL:HB    | 1.94                     | 0.49              |
| 48:DZ:41:VAL:HG13  | 48:DZ:42:GLU:N     | 2.28                     | 0.49              |
| 1:AA:1349:A:H62    | 1:AA:1373:G:H21    | 1.60                     | 0.49              |
| 1:AA:1434:A:C2'    | 1:AA:1435:G:H5'    | 2.43                     | 0.49              |
| 1:AA:506:G:O6      | 1:AA:525:C:N4      | 2.45                     | 0.49              |
| 2:AB:104:ASN:O     | 2:AB:105:PHE:C     | 2.51                     | 0.49              |
| 2:AB:123:ALA:O     | 2:AB:124:SER:HB2   | 2.13                     | 0.49              |
| 3:AC:8:ILE:O       | 3:AC:12:LEU:N      | 2.45                     | 0.49              |
| 4:AD:162:LEU:O     | 4:AD:165:MET:HB2   | 2.12                     | 0.49              |
| 5:AE:10:MET:HB2    | 5:AE:31:LEU:O      | 2.12                     | 0.49              |
| 5:AE:34:VAL:HG12   | 5:AE:35:GLY:N      | 2.27                     | 0.49              |
| 5:AE:59:GLY:O      | 5:AE:62:ALA:HB3    | 2.11                     | 0.49              |
| 6:AF:62:TRP:CD1    | 18:AR:35:ARG:NH1   | 2.81                     | 0.49              |
| 6:AF:77:ARG:O      | 6:AF:78:GLU:C      | 2.51                     | 0.49              |
| 7:AG:153:HIS:O     | 7:AG:154:TYR:HD2   | 1.95                     | 0.49              |
| 1:AA:942:G:H21     | 9:AI:124:GLN:HE22  | 1.56                     | 0.49              |
| 10:AJ:4:ILE:HA     | 10:AJ:100:THR:HG22 | 1.94                     | 0.49              |
| 10:AJ:46:ARG:HD3   | 14:AN:61:TRP:CH2   | 2.48                     | 0.49              |
| 10:AJ:81:THR:O     | 10:AJ:83:GLU:N     | 2.46                     | 0.49              |
| 15:AO:82:ILE:O     | 15:AO:86:GLY:N     | 2.44                     | 0.49              |
| 1:AA:376:G:O3'     | 16:AP:5:ARG:HD2    | 2.12                     | 0.49              |
| 1:AA:472:A:C4'     | 16:AP:80:PHE:O     | 2.58                     | 0.49              |
| 19:AS:49:ILE:HD12  | 19:AS:49:ILE:N     | 2.21                     | 0.49              |
| 23:AW:71:A:H2'     | 23:AW:72:G:O4'     | 2.13                     | 0.49              |
| 24:AX:4:G:H1'      | 24:AX:70:G:N2      | 2.28                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:AY:4:G:C2      | 25:AY:69:C:C2     | 3.00                     | 0.49              |
| 25:AY:5:G:H2'     | 25:AY:6:U:O4'     | 2.12                     | 0.49              |
| 52:B3:24:LYS:HE3  | 52:B3:24:LYS:HA   | 1.95                     | 0.49              |
| 27:BA:1711:C:O2'  | 27:BA:1712:C:H5'  | 2.12                     | 0.49              |
| 27:BA:2534:A:C5'  | 27:BA:2534:A:H8   | 2.25                     | 0.49              |
| 27:BA:402:A:C2'   | 27:BA:403:U:H5'   | 2.43                     | 0.49              |
| 27:BA:658:C:H2'   | 27:BA:659:C:C6    | 2.48                     | 0.49              |
| 27:BA:794:G:C6    | 27:BA:795:C:C4    | 3.01                     | 0.49              |
| 27:BA:833:U:H2'   | 27:BA:834:C:H6    | 1.77                     | 0.49              |
| 30:BD:186:HIS:CD2 | 30:BD:187:GLY:N   | 2.81                     | 0.49              |
| 30:BD:267:SER:C   | 30:BD:269:PHE:N   | 2.59                     | 0.49              |
| 31:BE:14:ILE:HD12 | 42:BT:14:TYR:OH   | 2.13                     | 0.49              |
| 32:BF:160:ASN:ND2 | 32:BF:162:LEU:CB  | 2.74                     | 0.49              |
| 27:BA:440:G:H22   | 32:BF:46:ARG:HH22 | 1.60                     | 0.49              |
| 33:BG:23:PHE:HB2  | 33:BG:25:TYR:CE2  | 2.47                     | 0.49              |
| 34:BH:156:ALA:O   | 34:BH:157:TYR:HB3 | 2.13                     | 0.49              |
| 35:BI:133:HIS:CD2 | 35:BI:133:HIS:N   | 2.78                     | 0.49              |
| 36:BN:85:ILE:HG21 | 36:BN:90:MET:HE3  | 1.94                     | 0.49              |
| 36:BN:90:MET:HB3  | 36:BN:98:VAL:HG22 | 1.94                     | 0.49              |
| 37:BO:119:PRO:HB2 | 42:BT:68:TYR:CE1  | 2.44                     | 0.49              |
| 37:BO:38:VAL:HG12 | 37:BO:39:ILE:H    | 1.78                     | 0.49              |
| 39:BQ:118:LEU:O   | 39:BQ:121:ALA:N   | 2.46                     | 0.49              |
| 40:BR:22:ARG:O    | 40:BR:24:GLN:N    | 2.46                     | 0.49              |
| 42:BT:28:VAL:CG1  | 42:BT:46:GLU:HB2  | 2.42                     | 0.49              |
| 43:BU:91:ASP:O    | 43:BU:92:ARG:C    | 2.51                     | 0.49              |
| 28:BB:75:G:C5'    | 48:BZ:35:LYS:HE2  | 2.41                     | 0.49              |
| 1:CA:1041:A:H2'   | 1:CA:1042:G:H8    | 1.75                     | 0.49              |
| 1:CA:1113:C:H2'   | 1:CA:1114:C:H6    | 1.77                     | 0.49              |
| 1:CA:532:A:H2     | 1:CA:1207:G:O4'   | 1.96                     | 0.49              |
| 1:CA:1407:C:O2    | 1:CA:1495:U:O2    | 2.30                     | 0.49              |
| 1:CA:390:C:O2'    | 16:CP:28:ARG:NH2  | 2.46                     | 0.49              |
| 1:CA:532:A:O2'    | 1:CA:533:A:H5''   | 2.13                     | 0.49              |
| 1:CA:945:G:C2     | 1:CA:946:A:C8     | 3.00                     | 0.49              |
| 3:CC:95:THR:O     | 3:CC:97:LYS:N     | 2.46                     | 0.49              |
| 4:CD:61:LYS:HE3   | 4:CD:206:PHE:CE2  | 2.48                     | 0.49              |
| 5:CE:109:ILE:O    | 5:CE:113:ALA:HB2  | 2.13                     | 0.49              |
| 1:CA:921:U:O2'    | 5:CE:19:MET:O     | 2.20                     | 0.49              |
| 1:CA:450:G:H5''   | 16:CP:41:PRO:O    | 2.13                     | 0.49              |
| 17:CQ:51:TYR:HE2  | 17:CQ:76:LEU:H    | 1.60                     | 0.49              |
| 20:CT:57:ARG:NH1  | 20:CT:57:ARG:HB2  | 2.28                     | 0.49              |
| 21:CU:20:LYS:HG2  | 21:CU:20:LYS:O    | 2.12                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:D0:23:VAL:HB    | 49:D0:26:TYR:HE2   | 1.77                     | 0.49              |
| 49:D0:41:ARG:HD2   | 49:D0:41:ARG:N     | 2.06                     | 0.49              |
| 49:D0:70:GLN:HG3   | 49:D0:80:HIS:CD2   | 2.48                     | 0.49              |
| 51:D2:22:GLU:HG3   | 51:D2:64:LEU:HD11  | 1.95                     | 0.49              |
| 52:D3:4:LEU:HD21   | 52:D3:56:VAL:CG1   | 2.43                     | 0.49              |
| 56:D7:19:ARG:HG3   | 56:D7:19:ARG:NH1   | 2.27                     | 0.49              |
| 27:DA:1252:G:C2    | 43:DU:33:ARG:HD2   | 2.47                     | 0.49              |
| 27:DA:1352:U:O2    | 27:DA:1570:A:H2    | 1.96                     | 0.49              |
| 27:DA:1366:A:H2'   | 27:DA:1367:A:O4'   | 2.13                     | 0.49              |
| 27:DA:139:G:H1     | 27:DA:142(A):C:H42 | 1.58                     | 0.49              |
| 27:DA:1771:C:C1'   | 27:DA:1786:A:C8    | 2.95                     | 0.49              |
| 27:DA:1849:G:C2    | 27:DA:1850:G:N7    | 2.80                     | 0.49              |
| 27:DA:2066:C:H2'   | 27:DA:2067:G:O5'   | 2.13                     | 0.49              |
| 27:DA:2100:G:H2'   | 27:DA:2101:G:H8    | 1.68                     | 0.49              |
| 27:DA:2249:U:N3    | 27:DA:2253:G:OP2   | 2.45                     | 0.49              |
| 27:DA:2508:G:H2'   | 27:DA:2509:G:H8    | 1.77                     | 0.49              |
| 27:DA:1782:C:N4    | 27:DA:2586:C:H42   | 2.07                     | 0.49              |
| 27:DA:2595:G:C2    | 27:DA:2599:G:C6    | 3.00                     | 0.49              |
| 27:DA:635:C:O2'    | 27:DA:636:G:H5'    | 2.12                     | 0.49              |
| 27:DA:77:C:H2'     | 27:DA:78:A:C8      | 2.47                     | 0.49              |
| 31:DE:97:LYS:O     | 31:DE:99:GLY:N     | 2.46                     | 0.49              |
| 32:DF:57:VAL:CG1   | 32:DF:58:ALA:N     | 2.76                     | 0.49              |
| 33:DG:111:LEU:O    | 33:DG:112:PRO:C    | 2.49                     | 0.49              |
| 33:DG:120:LEU:HD11 | 33:DG:179:PRO:HD2  | 1.95                     | 0.49              |
| 33:DG:5:VAL:H      | 33:DG:8:LYS:HB2    | 1.78                     | 0.49              |
| 34:DH:100:GLY:C    | 34:DH:102:ALA:H    | 2.15                     | 0.49              |
| 39:DQ:21:THR:HG22  | 39:DQ:22:LYS:H     | 1.77                     | 0.49              |
| 40:DR:12:ARG:HD3   | 40:DR:16:HIS:CE1   | 2.47                     | 0.49              |
| 41:DS:78:LEU:C     | 41:DS:80:LEU:H     | 2.14                     | 0.49              |
| 27:DA:1322:A:OP1   | 45:DW:11:ARG:HG3   | 2.13                     | 0.49              |
| 48:DZ:109:GLY:O    | 48:DZ:114:GLY:O    | 2.31                     | 0.49              |
| 1:AA:189(J):G:H2'  | 1:AA:189(K):U:C6   | 2.48                     | 0.49              |
| 1:AA:408:A:H4'     | 4:AD:112:VAL:HG21  | 1.94                     | 0.49              |
| 1:AA:782:A:C2'     | 1:AA:783:C:H5'     | 2.42                     | 0.49              |
| 1:AA:887:G:C2      | 1:AA:911:U:O2      | 2.66                     | 0.49              |
| 2:AB:28:PHE:CZ     | 2:AB:189:ASP:HA    | 2.47                     | 0.49              |
| 5:AE:71:LEU:HD21   | 5:AE:115:VAL:HG22  | 1.95                     | 0.49              |
| 13:AM:11:ARG:HB3   | 13:AM:12:ASN:OD1   | 2.13                     | 0.49              |
| 13:AM:7:VAL:O      | 13:AM:8:GLU:C      | 2.51                     | 0.49              |
| 16:AP:44:THR:O     | 16:AP:45:THR:HB    | 2.13                     | 0.49              |
| 17:AQ:10:VAL:CG2   | 17:AQ:21:VAL:HG22  | 2.43                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:AW:1:U:H2'      | 23:AW:1:U:O2       | 2.13                     | 0.49              |
| 45:BW:38:TYR:HH    | 54:B5:47:PRO:HG3   | 1.75                     | 0.49              |
| 27:BA:1273:U:C6    | 27:BA:1273:U:C5'   | 2.89                     | 0.49              |
| 27:BA:1558:A:HO2'  | 27:BA:1559:G:P     | 2.34                     | 0.49              |
| 27:BA:2111:C:C5    | 27:BA:2145:C:N3    | 2.81                     | 0.49              |
| 27:BA:2713:A:OP2   | 27:BA:2713:A:H4'   | 2.11                     | 0.49              |
| 27:BA:2816:C:O2    | 27:BA:2831:G:C2    | 2.66                     | 0.49              |
| 27:BA:2850:A:N1    | 27:BA:2851:A:C5    | 2.81                     | 0.49              |
| 27:BA:374:A:C8     | 27:BA:375:C:C5     | 3.01                     | 0.49              |
| 27:BA:511:U:H5     | 27:BA:512:G:C5     | 2.31                     | 0.49              |
| 27:BA:564:C:O2'    | 27:BA:565:C:H5'    | 2.13                     | 0.49              |
| 27:BA:757:U:O2'    | 27:BA:758:C:H5'    | 2.13                     | 0.49              |
| 27:BA:825:C:O2'    | 38:BP:55:ARG:HD3   | 2.12                     | 0.49              |
| 27:BA:914:C:H2'    | 27:BA:915:C:O5'    | 2.12                     | 0.49              |
| 30:BD:131:LEU:HD13 | 30:BD:136:ILE:HD11 | 1.95                     | 0.49              |
| 31:BE:132:HIS:HD2  | 31:BE:135:HIS:CE1  | 2.30                     | 0.49              |
| 27:BA:674:G:P      | 32:BF:54:ARG:HH22  | 2.36                     | 0.49              |
| 33:BG:51:ARG:NH1   | 33:BG:53:LEU:HD21  | 2.27                     | 0.49              |
| 34:BH:10:PRO:CG    | 34:BH:50:VAL:N     | 2.75                     | 0.49              |
| 37:BO:106:LEU:C    | 37:BO:108:GLU:N    | 2.66                     | 0.49              |
| 27:BA:245:G:O5'    | 38:BP:73:GLY:HA2   | 2.13                     | 0.49              |
| 39:BQ:16:ARG:CG    | 39:BQ:17:LEU:N     | 2.76                     | 0.49              |
| 40:BR:50:HIS:HD2   | 40:BR:51:LEU:HD12  | 1.78                     | 0.49              |
| 43:BU:14:HIS:CD2   | 43:BU:32:PHE:CB    | 2.95                     | 0.49              |
| 27:BA:1011:G:OP2   | 43:BU:66:ASN:OD1   | 2.31                     | 0.49              |
| 48:BZ:58:LEU:O     | 48:BZ:60:LEU:HD23  | 2.12                     | 0.49              |
| 48:BZ:70:VAL:HG22  | 48:BZ:87:PHE:HE2   | 1.75                     | 0.49              |
| 1:CA:1363:C:H5'    | 1:CA:1363(A):A:O5' | 2.13                     | 0.49              |
| 1:CA:36:C:OP1      | 12:CL:120:LYS:NZ   | 2.36                     | 0.49              |
| 1:CA:791:G:H8      | 1:CA:791:G:O5'     | 1.96                     | 0.49              |
| 2:CB:120:ALA:C     | 2:CB:122:PHE:H     | 2.15                     | 0.49              |
| 2:CB:132:LYS:HA    | 2:CB:135:GLN:CG    | 2.42                     | 0.49              |
| 2:CB:37:ASN:O      | 2:CB:39:ILE:HG13   | 2.12                     | 0.49              |
| 3:CC:110:ASN:O     | 3:CC:111:LEU:HD23  | 2.13                     | 0.49              |
| 3:CC:165:THR:HG22  | 3:CC:165:THR:O     | 2.13                     | 0.49              |
| 3:CC:35:GLU:O      | 3:CC:39:ILE:HG13   | 2.12                     | 0.49              |
| 4:CD:79:PHE:HD2    | 4:CD:80:GLU:N      | 2.10                     | 0.49              |
| 11:CK:123:LYS:CA   | 11:CK:126:ARG:HG3  | 2.42                     | 0.49              |
| 14:CN:24:CYS:O     | 14:CN:25:VAL:C     | 2.52                     | 0.49              |
| 16:CP:22:THR:OG1   | 16:CP:23:ASP:N     | 2.46                     | 0.49              |
| 49:D0:27:GLU:HB2   | 49:D0:69:PHE:HD1   | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 58:D9:26:ILE:N    | 58:D9:26:ILE:HD12 | 2.27                     | 0.49              |
| 27:DA:1175:U:O3'  | 27:DA:1176:G:H3'  | 2.13                     | 0.49              |
| 27:DA:1287:A:C5   | 27:DA:1288:U:C4   | 3.01                     | 0.49              |
| 27:DA:1479:G:H5'  | 27:DA:1558:A:H2   | 1.78                     | 0.49              |
| 27:DA:2524:G:H2'  | 27:DA:2741:A:C2   | 2.48                     | 0.49              |
| 27:DA:904:C:H2'   | 27:DA:905:U:C5'   | 2.34                     | 0.49              |
| 27:DA:965:C:H2'   | 27:DA:966:G:H5'   | 1.94                     | 0.49              |
| 31:DE:69:LYS:C    | 31:DE:71:GLY:N    | 2.66                     | 0.49              |
| 31:DE:71:GLY:O    | 31:DE:72:VAL:HB   | 2.13                     | 0.49              |
| 32:DF:67:GLN:O    | 32:DF:68:LYS:HB2  | 2.13                     | 0.49              |
| 33:DG:77:ILE:CG2  | 33:DG:79:ASN:HB2  | 2.43                     | 0.49              |
| 33:DG:91:ARG:HD2  | 33:DG:92:VAL:N    | 2.28                     | 0.49              |
| 35:DI:13:GLY:O    | 35:DI:17:GLN:OE1  | 2.31                     | 0.49              |
| 36:DN:2:LYS:O     | 36:DN:4:TYR:CZ    | 2.65                     | 0.49              |
| 36:DN:42:TRP:HA   | 36:DN:42:TRP:HE3  | 1.77                     | 0.49              |
| 39:DQ:51:ARG:CB   | 39:DQ:51:ARG:HH11 | 2.24                     | 0.49              |
| 27:DA:1654:A:OP2  | 40:DR:3:HIS:CD2   | 2.66                     | 0.49              |
| 40:DR:77:ARG:O    | 40:DR:79:LEU:N    | 2.46                     | 0.49              |
| 41:DS:25:ARG:HH12 | 41:DS:40:ILE:CD1  | 2.26                     | 0.49              |
| 41:DS:68:GLN:O    | 41:DS:71:ARG:HB2  | 2.13                     | 0.49              |
| 41:DS:87:PHE:HZ   | 41:DS:99:LYS:CG   | 2.26                     | 0.49              |
| 46:DX:4:ALA:HB3   | 46:DX:5:TYR:CD1   | 2.47                     | 0.49              |
| 46:DX:64:LYS:NZ   | 46:DX:73:ARG:HH22 | 2.11                     | 0.49              |
| 1:AA:1004:A:C5'   | 1:AA:1025:U:H3    | 2.16                     | 0.48              |
| 1:AA:1145:C:H4'   | 1:AA:1146:A:C5'   | 2.43                     | 0.48              |
| 1:AA:1146:A:O2'   | 1:AA:1147:C:H5''  | 2.13                     | 0.48              |
| 1:AA:235:C:C5'    | 17:AQ:70:ARG:HG2  | 2.44                     | 0.48              |
| 1:AA:115:G:C2     | 1:AA:289:G:N7     | 2.81                     | 0.48              |
| 1:AA:376:G:O2'    | 1:AA:377:G:H5'    | 2.12                     | 0.48              |
| 1:AA:533:A:OP1    | 1:AA:533:A:H3'    | 2.13                     | 0.48              |
| 1:AA:655:A:H2'    | 1:AA:656:C:C6     | 2.47                     | 0.48              |
| 1:AA:818:G:C3'    | 1:AA:819:A:H5''   | 2.43                     | 0.48              |
| 1:AA:922:G:H2'    | 1:AA:923:A:C8     | 2.48                     | 0.48              |
| 2:AB:144:ARG:HG3  | 2:AB:145:LEU:H    | 1.78                     | 0.48              |
| 9:AI:93:ARG:C     | 9:AI:95:LYS:H     | 2.16                     | 0.48              |
| 14:AN:43:CYS:O    | 14:AN:47:LEU:HG   | 2.12                     | 0.48              |
| 15:AO:17:ARG:NH1  | 15:AO:17:ARG:HG3  | 2.24                     | 0.48              |
| 16:AP:8:ARG:O     | 16:AP:9:PHE:CD1   | 2.66                     | 0.48              |
| 20:AT:79:ARG:NH2  | 20:AT:80:ARG:NH2  | 2.60                     | 0.48              |
| 54:B5:52:TYR:HD1  | 54:B5:52:TYR:O    | 1.96                     | 0.48              |
| 58:B9:29:ASN:N    | 58:B9:29:ASN:ND2  | 2.44                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1043:C:O2'  | 27:BA:1044:G:C8    | 2.57                     | 0.48              |
| 27:BA:1225:G:O2'  | 27:BA:1226:A:H5'   | 2.12                     | 0.48              |
| 27:BA:1451:C:O2'  | 27:BA:1457:A:N6    | 2.45                     | 0.48              |
| 27:BA:1469:A:C2   | 27:BA:1524:G:C2    | 3.01                     | 0.48              |
| 27:BA:1887:C:H3'  | 27:BA:1888:G:H5''  | 1.95                     | 0.48              |
| 27:BA:1948:G:C2'  | 27:BA:1949:G:H5'   | 2.43                     | 0.48              |
| 27:BA:2078:C:H2'  | 27:BA:2079:U:C6    | 2.48                     | 0.48              |
| 27:BA:2125:G:N2   | 27:BA:2174:C:N4    | 2.61                     | 0.48              |
| 27:BA:2270:G:H2'  | 27:BA:2271:G:C8    | 2.47                     | 0.48              |
| 27:BA:25:U:H2'    | 27:BA:26:G:O5'     | 2.12                     | 0.48              |
| 27:BA:2776:A:H4'  | 27:BA:2777:G:O5'   | 2.13                     | 0.48              |
| 27:BA:2837:G:C6   | 27:BA:2838:G:N7    | 2.80                     | 0.48              |
| 27:BA:56:A:C2     | 27:BA:57:C:C2      | 3.01                     | 0.48              |
| 27:BA:66:C:C2'    | 27:BA:67:U:H5'     | 2.42                     | 0.48              |
| 27:BA:709:U:C2    | 27:BA:710:G:C8     | 3.00                     | 0.48              |
| 27:BA:764:A:C5    | 30:BD:209:ALA:HB1  | 2.47                     | 0.48              |
| 29:BC:195:ALA:O   | 29:BC:197:GLU:N    | 2.46                     | 0.48              |
| 31:BE:1:MET:HB2   | 31:BE:83:ASP:O     | 2.13                     | 0.48              |
| 32:BF:53:THR:O    | 32:BF:56:GLU:N     | 2.44                     | 0.48              |
| 33:BG:71:THR:O    | 33:BG:89:GLY:HA3   | 2.12                     | 0.48              |
| 34:BH:68:THR:O    | 34:BH:70:THR:O     | 2.31                     | 0.48              |
| 35:BI:115:ALA:CB  | 35:BI:129:THR:OG1  | 2.58                     | 0.48              |
| 35:BI:90:GLY:O    | 35:BI:91:SER:C     | 2.52                     | 0.48              |
| 36:BN:35:ARG:C    | 36:BN:37:LYS:H     | 2.16                     | 0.48              |
| 41:BS:54:LEU:C    | 41:BS:56:LEU:N     | 2.67                     | 0.48              |
| 42:BT:89:VAL:HB   | 42:BT:91:ARG:NE    | 2.06                     | 0.48              |
| 43:BU:89:GLU:H    | 43:BU:89:GLU:HG2   | 1.39                     | 0.48              |
| 43:BU:96:ALA:C    | 43:BU:98:LEU:H     | 2.16                     | 0.48              |
| 44:BV:35:LEU:CB   | 44:BV:37:VAL:HG23  | 2.40                     | 0.48              |
| 48:BZ:51:SER:OG   | 48:BZ:52:ILE:N     | 2.46                     | 0.48              |
| 1:CA:1002:G:H21   | 1:CA:1003:G:H1'    | 1.74                     | 0.48              |
| 1:CA:1157:A:C6    | 1:CA:1180:A:C5     | 3.01                     | 0.48              |
| 1:CA:1292:U:H2'   | 1:CA:1293:G:H8     | 1.78                     | 0.48              |
| 1:CA:1363(A):A:N3 | 1:CA:1363(A):A:H2' | 2.27                     | 0.48              |
| 1:CA:263:A:H2'    | 1:CA:264:U:H6      | 1.77                     | 0.48              |
| 1:CA:270:A:C6     | 1:CA:271:C:N3      | 2.80                     | 0.48              |
| 1:CA:742:G:C5'    | 15:CO:58:MET:CE    | 2.86                     | 0.48              |
| 1:CA:830:G:H1     | 1:CA:856:C:N4      | 2.10                     | 0.48              |
| 3:CC:90:GLU:HA    | 3:CC:93:LYS:HB2    | 1.93                     | 0.48              |
| 4:CD:10:ARG:O     | 4:CD:13:ARG:HB2    | 2.13                     | 0.48              |
| 6:CF:43:LEU:H     | 6:CF:43:LEU:CD1    | 2.24                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:CK:110:ASP:O    | 18:CR:84:LYS:HB3    | 2.12                     | 0.48              |
| 1:CA:36:C:H5''     | 12:CL:120:LYS:HD3   | 1.93                     | 0.48              |
| 16:CP:67:THR:HB    | 16:CP:70:ALA:H      | 1.77                     | 0.48              |
| 16:CP:82:GLN:O     | 16:CP:83:GLU:HG2    | 2.12                     | 0.48              |
| 17:CQ:82:MET:O     | 17:CQ:86:GLU:HG2    | 2.13                     | 0.48              |
| 1:CA:958:A:N7      | 19:CS:55:LYS:HD2    | 2.28                     | 0.48              |
| 1:CA:1226:C:OP1    | 19:CS:81:ARG:NH2    | 2.44                     | 0.48              |
| 24:CX:4:G:O2'      | 24:CX:5:G:H5'       | 2.13                     | 0.48              |
| 49:D0:56:ASP:O     | 49:D0:57:PHE:HB2    | 2.13                     | 0.48              |
| 52:D3:16:PRO:HB2   | 52:D3:19:GLN:HG3    | 1.93                     | 0.48              |
| 53:D4:40:ILE:N     | 53:D4:40:ILE:HD12   | 2.27                     | 0.48              |
| 27:DA:1721:G:O6    | 27:DA:1739:U:H5'    | 2.13                     | 0.48              |
| 27:DA:1844:C:H2'   | 27:DA:1845:G:O4'    | 2.13                     | 0.48              |
| 27:DA:1861:G:H1    | 27:DA:1881:C:H42    | 1.61                     | 0.48              |
| 27:DA:2307:G:H3'   | 27:DA:2308:G:C5'    | 2.43                     | 0.48              |
| 27:DA:237:C:H6     | 27:DA:237:C:O5'     | 1.96                     | 0.48              |
| 27:DA:2469:A:N6    | 27:DA:2470:G:C2     | 2.81                     | 0.48              |
| 27:DA:2579:C:O2'   | 31:DE:131:ALA:CB    | 2.61                     | 0.48              |
| 27:DA:271(M):G:C2' | 27:DA:271(N):U:H5'' | 2.39                     | 0.48              |
| 27:DA:321:G:O2'    | 27:DA:322:A:OP1     | 2.23                     | 0.48              |
| 27:DA:346:A:C2'    | 27:DA:347:A:H5'     | 2.43                     | 0.48              |
| 27:DA:37:C:C2      | 27:DA:38:A:C8       | 3.00                     | 0.48              |
| 30:DD:67:PHE:CE1   | 30:DD:157:ARG:NH2   | 2.81                     | 0.48              |
| 30:DD:176:ARG:O    | 30:DD:177:LEU:HD23  | 2.13                     | 0.48              |
| 30:DD:265:PRO:C    | 30:DD:267:SER:N     | 2.65                     | 0.48              |
| 31:DE:1:MET:O      | 31:DE:2:LYS:C       | 2.52                     | 0.48              |
| 32:DF:66:PRO:O     | 32:DF:67:GLN:C      | 2.52                     | 0.48              |
| 36:DN:3:THR:O      | 36:DN:3:THR:HG22    | 2.13                     | 0.48              |
| 37:DO:1:MET:HE2    | 37:DO:1:MET:N       | 2.28                     | 0.48              |
| 37:DO:4:PRO:O      | 37:DO:5:GLN:CB      | 2.61                     | 0.48              |
| 39:DQ:118:LEU:HD13 | 39:DQ:131:ILE:HG12  | 1.94                     | 0.48              |
| 40:DR:4:LEU:C      | 40:DR:5:LYS:HD2     | 2.33                     | 0.48              |
| 41:DS:16:ASN:C     | 41:DS:20:ARG:NH2    | 2.65                     | 0.48              |
| 43:DU:55:ARG:HA    | 43:DU:58:ARG:CB     | 2.23                     | 0.48              |
| 44:DV:19:LYS:HB2   | 44:DV:96:ILE:CG1    | 2.39                     | 0.48              |
| 45:DW:4:LYS:HG2    | 45:DW:106:ILE:HG21  | 1.94                     | 0.48              |
| 1:AA:115:G:H1'     | 1:AA:116:A:N7       | 2.27                     | 0.48              |
| 1:AA:1305:G:O2'    | 1:AA:1306:A:O5'     | 2.30                     | 0.48              |
| 1:AA:189(I):G:HO2' | 1:AA:189(J):G:H8    | 1.59                     | 0.48              |
| 1:AA:511:C:O2'     | 1:AA:512:U:H6       | 1.95                     | 0.48              |
| 1:AA:829:G:O2'     | 1:AA:830:G:H5'      | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:939:G:OP1     | 7:AG:102:ARG:NH2   | 2.46                     | 0.48              |
| 1:AA:960:U:O2'     | 1:AA:1223:C:C4'    | 2.61                     | 0.48              |
| 3:AC:139:GLN:O     | 3:AC:143:GLU:CB    | 2.61                     | 0.48              |
| 7:AG:154:TYR:C     | 7:AG:156:TRP:H     | 2.15                     | 0.48              |
| 1:AA:875:C:O2'     | 8:AH:14:ARG:HD2    | 2.13                     | 0.48              |
| 9:AI:53:VAL:HG12   | 9:AI:92:TYR:HD2    | 1.77                     | 0.48              |
| 9:AI:24:GLY:HA2    | 9:AI:59:PHE:O      | 2.13                     | 0.48              |
| 10:AJ:22:LYS:HZ2   | 10:AJ:23:ILE:HA    | 1.79                     | 0.48              |
| 12:AL:123:LYS:CD   | 12:AL:124:GLU:H    | 2.25                     | 0.48              |
| 1:AA:1225:A:H5''   | 13:AM:103:THR:HG21 | 1.96                     | 0.48              |
| 13:AM:16:ASP:OD2   | 13:AM:17:VAL:HG23  | 2.13                     | 0.48              |
| 1:AA:740:U:H4'     | 15:AO:39:LEU:CD2   | 2.43                     | 0.48              |
| 16:AP:21:VAL:O     | 16:AP:32:TYR:HB2   | 2.13                     | 0.48              |
| 19:AS:29:ARG:O     | 19:AS:31:ILE:N     | 2.46                     | 0.48              |
| 20:AT:57:ARG:HB2   | 20:AT:57:ARG:NH1   | 2.27                     | 0.48              |
| 50:B1:86:SER:O     | 50:B1:90:ILE:HG12  | 2.12                     | 0.48              |
| 57:B8:6:THR:HG22   | 57:B8:63:PRO:CD    | 2.43                     | 0.48              |
| 27:BA:154(A):C:O4' | 27:BA:154(A):C:O2  | 2.31                     | 0.48              |
| 27:BA:2238:G:N3    | 27:BA:2238:G:H2'   | 2.28                     | 0.48              |
| 27:BA:239:U:O4'    | 27:BA:621:A:H2     | 1.95                     | 0.48              |
| 27:BA:2476:A:C2    | 27:BA:2477:C:C6    | 3.00                     | 0.48              |
| 23:AW:74:C:H4'     | 27:BA:2573:C:N4    | 2.29                     | 0.48              |
| 27:BA:2701:C:C2'   | 27:BA:2702:U:H5''  | 2.40                     | 0.48              |
| 27:BA:271(G):C:C2  | 27:BA:271(H):G:N7  | 2.81                     | 0.48              |
| 27:BA:2832:U:O4    | 27:BA:2884:U:H5''  | 2.13                     | 0.48              |
| 27:BA:663:G:C5     | 27:BA:664:C:C5     | 3.01                     | 0.48              |
| 27:BA:65:C:H2'     | 27:BA:66:C:H6      | 1.79                     | 0.48              |
| 27:BA:680:G:O2'    | 27:BA:681:G:H5'    | 2.12                     | 0.48              |
| 27:BA:793:A:OP2    | 27:BA:2072:G:H5'   | 2.13                     | 0.48              |
| 28:BB:105:A:N7     | 28:BB:106:G:C8     | 2.81                     | 0.48              |
| 28:BB:11:C:H3'     | 28:BB:12:C:H6      | 1.77                     | 0.48              |
| 29:BC:20:TYR:CD2   | 29:BC:21:THR:N     | 2.78                     | 0.48              |
| 30:BD:158:ALA:O    | 30:BD:196:VAL:HG11 | 2.13                     | 0.48              |
| 31:BE:51:PHE:CE1   | 31:BE:52:LEU:HD13  | 2.48                     | 0.48              |
| 33:BG:53:LEU:H     | 33:BG:53:LEU:HD22  | 1.77                     | 0.48              |
| 34:BH:94:TYR:CE1   | 34:BH:108:GLY:N    | 2.80                     | 0.48              |
| 34:BH:10:PRO:CG    | 34:BH:50:VAL:O     | 2.54                     | 0.48              |
| 35:BI:12:LEU:HD12  | 35:BI:19:VAL:CG1   | 2.38                     | 0.48              |
| 35:BI:4:ILE:HG12   | 35:BI:18:VAL:CG2   | 2.43                     | 0.48              |
| 46:BX:28:PHE:CE2   | 46:BX:92:LEU:HD11  | 2.48                     | 0.48              |
| 1:CA:1252:A:C2     | 1:CA:1253:G:C4     | 3.01                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1267:C:O2    | 1:CA:1267:C:C2'   | 2.57                     | 0.48              |
| 1:CA:153:C:H2'    | 1:CA:154:C:C6     | 2.48                     | 0.48              |
| 1:CA:159:G:H21    | 1:CA:161:A:H3'    | 1.77                     | 0.48              |
| 1:CA:189(K):U:O5' | 1:CA:189(K):U:H6  | 1.97                     | 0.48              |
| 1:CA:532:A:C2'    | 1:CA:533:A:H5'    | 2.42                     | 0.48              |
| 1:CA:515:G:N2     | 1:CA:537:G:C4     | 2.81                     | 0.48              |
| 1:CA:933:G:OP1    | 7:CG:4:ARG:HD2    | 2.13                     | 0.48              |
| 2:CB:118:LEU:HD11 | 2:CB:141:GLU:CD   | 2.33                     | 0.48              |
| 2:CB:55:PHE:HA    | 2:CB:58:ILE:CG1   | 2.31                     | 0.48              |
| 4:CD:173:TRP:HB2  | 4:CD:187:ARG:O    | 2.13                     | 0.48              |
| 4:CD:25:ARG:O     | 4:CD:27:TYR:N     | 2.46                     | 0.48              |
| 4:CD:2:GLY:C      | 4:CD:4:TYR:H      | 2.16                     | 0.48              |
| 4:CD:70:ILE:HD12  | 4:CD:100:ARG:HD2  | 1.94                     | 0.48              |
| 8:CH:61:VAL:O     | 8:CH:63:LEU:HD13  | 2.12                     | 0.48              |
| 10:CJ:46:ARG:HG2  | 10:CJ:64:GLU:HB3  | 1.94                     | 0.48              |
| 12:CL:52:VAL:CG1  | 12:CL:53:ALA:N    | 2.76                     | 0.48              |
| 12:CL:83:ARG:HH21 | 12:CL:96:HIS:CG   | 2.31                     | 0.48              |
| 20:CT:54:LYS:HA   | 20:CT:57:ARG:CZ   | 2.41                     | 0.48              |
| 21:CU:22:ARG:H    | 21:CU:23:PRO:HD3  | 1.78                     | 0.48              |
| 27:DA:1006:C:O2'  | 27:DA:1007:C:H5'  | 2.13                     | 0.48              |
| 27:DA:1011:G:C6   | 27:DA:1013:C:C4   | 3.01                     | 0.48              |
| 27:DA:1212:G:N3   | 27:DA:1236:G:C2   | 2.82                     | 0.48              |
| 27:DA:1257:C:O2'  | 32:DF:83:PHE:O    | 2.31                     | 0.48              |
| 27:DA:1309:G:H5'' | 56:D7:9:ARG:HG3   | 1.95                     | 0.48              |
| 27:DA:1341:U:C5   | 27:DA:1395:A:H2   | 2.31                     | 0.48              |
| 27:DA:1462:C:H2'  | 27:DA:1463:C:C6   | 2.47                     | 0.48              |
| 27:DA:149:A:H2'   | 27:DA:150:C:O5'   | 2.12                     | 0.48              |
| 27:DA:1505:C:O2   | 27:DA:1505:C:O4'  | 2.28                     | 0.48              |
| 27:DA:1429:G:C8   | 27:DA:1568:G:C5   | 3.01                     | 0.48              |
| 27:DA:1844:C:C2   | 27:DA:1845:G:C8   | 3.01                     | 0.48              |
| 27:DA:2065:C:N4   | 27:DA:2066:C:N4   | 2.61                     | 0.48              |
| 27:DA:2081:C:O2'  | 27:DA:2082:A:H5'  | 2.12                     | 0.48              |
| 27:DA:2111:C:H42  | 27:DA:2147:G:H22  | 1.60                     | 0.48              |
| 27:DA:2432:A:N6   | 27:DA:2433:A:C6   | 2.81                     | 0.48              |
| 27:DA:2461:C:C5   | 27:DA:2462:U:H5   | 2.32                     | 0.48              |
| 27:DA:2840:C:H2'  | 27:DA:2841:C:H6   | 1.77                     | 0.48              |
| 27:DA:407:G:H2'   | 27:DA:408:G:H8    | 1.74                     | 0.48              |
| 27:DA:819:A:N1    | 27:DA:820:A:C4    | 2.81                     | 0.48              |
| 27:DA:822:U:O2'   | 27:DA:823:G:H5'   | 2.13                     | 0.48              |
| 27:DA:1491:G:O2'  | 30:DD:101:GLU:HB2 | 2.13                     | 0.48              |
| 27:DA:2580:U:P    | 31:DE:131:ALA:HB2 | 2.54                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DF:54:ARG:CZ    | 32:DF:80:ALA:HB2  | 2.43                     | 0.48              |
| 33:DG:175:LEU:HD12 | 33:DG:175:LEU:H   | 1.78                     | 0.48              |
| 37:DO:9:GLU:O      | 37:DO:83:ALA:HA   | 2.13                     | 0.48              |
| 40:DR:25:ALA:C     | 40:DR:27:SER:N    | 2.65                     | 0.48              |
| 40:DR:28:LEU:HA    | 40:DR:34:ILE:CG1  | 2.43                     | 0.48              |
| 40:DR:38:VAL:CB    | 40:DR:39:PRO:CD   | 2.91                     | 0.48              |
| 40:DR:99:LYS:NZ    | 54:D5:43:HIS:HB3  | 2.27                     | 0.48              |
| 42:DT:101:PHE:O    | 42:DT:102:ILE:C   | 2.51                     | 0.48              |
| 42:DT:35:LYS:NZ    | 42:DT:41:ARG:HH21 | 2.11                     | 0.48              |
| 44:DV:19:LYS:HE2   | 44:DV:19:LYS:HA   | 1.95                     | 0.48              |
| 44:DV:28:GLU:O     | 44:DV:29:PRO:O    | 2.31                     | 0.48              |
| 44:DV:71:LEU:HD11  | 44:DV:84:LYS:HE2  | 1.94                     | 0.48              |
| 44:DV:80:GLN:HA    | 44:DV:80:GLN:HE21 | 1.78                     | 0.48              |
| 45:DW:31:GLU:HA    | 45:DW:31:GLU:OE2  | 2.13                     | 0.48              |
| 27:DA:2012:G:O3'   | 45:DW:96:ILE:CD1  | 2.61                     | 0.48              |
| 47:DY:26:LYS:HG2   | 47:DY:27:VAL:HG23 | 1.95                     | 0.48              |
| 47:DY:28:LYS:C     | 47:DY:38:ILE:HB   | 2.34                     | 0.48              |
| 47:DY:39:VAL:O     | 47:DY:40:GLU:CD   | 2.52                     | 0.48              |
| 1:AA:1102:A:H2'    | 1:AA:1103:C:H6    | 1.77                     | 0.48              |
| 1:AA:1344:C:C2'    | 1:AA:1345:U:H5'   | 2.43                     | 0.48              |
| 1:AA:1381:U:H5''   | 1:AA:1381:U:C6    | 2.49                     | 0.48              |
| 1:AA:428:G:O4'     | 1:AA:430:A:C8     | 2.66                     | 0.48              |
| 1:AA:451:A:H61     | 1:AA:481:G:H5'    | 1.77                     | 0.48              |
| 2:AB:19:HIS:CG     | 2:AB:20:GLU:N     | 2.81                     | 0.48              |
| 2:AB:204:ASN:ND2   | 2:AB:206:ASP:H    | 2.10                     | 0.48              |
| 3:AC:5:ILE:O       | 3:AC:5:ILE:CD1    | 2.60                     | 0.48              |
| 6:AF:75:LEU:O      | 6:AF:77:ARG:N     | 2.46                     | 0.48              |
| 8:AH:50:ARG:HA     | 8:AH:59:LEU:HD23  | 1.94                     | 0.48              |
| 10:AJ:63:PHE:N     | 10:AJ:63:PHE:CD2  | 2.82                     | 0.48              |
| 13:AM:20:THR:O     | 13:AM:22:ILE:N    | 2.39                     | 0.48              |
| 15:AO:26:GLU:CD    | 15:AO:77:ARG:HD2  | 2.33                     | 0.48              |
| 17:AQ:68:ARG:N     | 17:AQ:70:ARG:HH12 | 2.11                     | 0.48              |
| 18:AR:64:ARG:HG3   | 18:AR:64:ARG:HH11 | 1.78                     | 0.48              |
| 27:BA:2330:G:N2    | 49:B0:42:GLY:HA2  | 2.29                     | 0.48              |
| 49:B0:50:ASN:O     | 49:B0:81:VAL:HG21 | 2.13                     | 0.48              |
| 50:B1:11:ARG:HB2   | 50:B1:12:PRO:HD2  | 1.95                     | 0.48              |
| 52:B3:8:LEU:HD13   | 52:B3:31:LEU:CD2  | 2.43                     | 0.48              |
| 55:B6:28:ARG:NH1   | 55:B6:28:ARG:HG2  | 2.28                     | 0.48              |
| 27:BA:1605:C:C5    | 27:BA:1606:G:C5   | 3.01                     | 0.48              |
| 27:BA:1814:G:C6    | 27:BA:1815:A:C6   | 3.02                     | 0.48              |
| 27:BA:2075:U:H2'   | 27:BA:2238:G:N2   | 2.28                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2348:U:H2'  | 27:BA:2349:G:H5''  | 1.95                     | 0.48              |
| 27:BA:251:A:H2'   | 27:BA:252:G:O4'    | 2.12                     | 0.48              |
| 27:BA:2686:G:H2'  | 27:BA:2687:U:O4'   | 2.13                     | 0.48              |
| 27:BA:356:G:H2'   | 27:BA:356:G:N3     | 2.28                     | 0.48              |
| 27:BA:263:C:O2'   | 27:BA:429:A:N3     | 2.43                     | 0.48              |
| 27:BA:486:C:H2'   | 27:BA:487:C:H6     | 1.77                     | 0.48              |
| 27:BA:670:A:H8    | 27:BA:670:A:O5'    | 1.93                     | 0.48              |
| 27:BA:671:C:C6    | 27:BA:671:C:C5'    | 2.96                     | 0.48              |
| 27:BA:788:A:OP1   | 27:BA:791:C:N4     | 2.45                     | 0.48              |
| 27:BA:907:U:H5'   | 39:BQ:23:GLY:HA3   | 1.95                     | 0.48              |
| 27:BA:729:G:C6    | 30:BD:208:LYS:HB2  | 2.48                     | 0.48              |
| 33:BG:114:ILE:O   | 33:BG:115:ARG:O    | 2.31                     | 0.48              |
| 33:BG:23:PHE:CD1  | 33:BG:23:PHE:N     | 2.81                     | 0.48              |
| 34:BH:118:PRO:HG3 | 34:BH:144:VAL:HG21 | 1.94                     | 0.48              |
| 35:BI:1:MET:C     | 35:BI:20:ASP:HB2   | 2.33                     | 0.48              |
| 36:BN:94:HIS:H    | 36:BN:95:PRO:HD2   | 1.78                     | 0.48              |
| 38:BP:50:ARG:HD3  | 57:B8:7:HIS:CD2    | 2.48                     | 0.48              |
| 39:BQ:20:ALA:O    | 39:BQ:98:LYS:HB2   | 2.13                     | 0.48              |
| 39:BQ:62:GLY:O    | 39:BQ:63:LYS:O     | 2.30                     | 0.48              |
| 39:BQ:12:GLN:HG3  | 39:BQ:73:PRO:HD2   | 1.95                     | 0.48              |
| 41:BS:92:TYR:C    | 41:BS:94:TYR:N     | 2.66                     | 0.48              |
| 43:BU:66:ASN:O    | 43:BU:70:ARG:HB2   | 2.13                     | 0.48              |
| 45:BW:22:ASP:HA   | 45:BW:25:ARG:HH12  | 1.78                     | 0.48              |
| 45:BW:57:ASN:N    | 45:BW:57:ASN:HD22  | 2.10                     | 0.48              |
| 48:BZ:100:PRO:O   | 48:BZ:101:LEU:HD12 | 2.13                     | 0.48              |
| 1:CA:1101:A:H1'   | 1:CA:1102:A:O4'    | 2.13                     | 0.48              |
| 1:CA:131:C:O2     | 1:CA:262:A:H2      | 1.96                     | 0.48              |
| 1:CA:1305:G:N2    | 1:CA:1331:G:C2'    | 2.72                     | 0.48              |
| 1:CA:1478:C:C2    | 1:CA:1479:C:C5     | 3.01                     | 0.48              |
| 1:CA:162:A:H8     | 1:CA:162:A:O5'     | 1.97                     | 0.48              |
| 1:CA:444:C:H2'    | 1:CA:445:G:C8      | 2.48                     | 0.48              |
| 1:CA:702:A:H4'    | 1:CA:703:G:OP2     | 2.12                     | 0.48              |
| 1:CA:797:C:O2'    | 1:CA:798:G:H5'     | 2.13                     | 0.48              |
| 1:CA:834:C:H2'    | 1:CA:835:U:O5'     | 2.12                     | 0.48              |
| 7:CG:143:ARG:NH2  | 25:CY:41:G:H5'     | 2.28                     | 0.48              |
| 10:CJ:22:LYS:HZ2  | 10:CJ:23:ILE:HG12  | 1.77                     | 0.48              |
| 14:CN:24:CYS:O    | 14:CN:27:CYS:O     | 2.31                     | 0.48              |
| 17:CQ:21:VAL:HG12 | 17:CQ:23:VAL:HG22  | 1.95                     | 0.48              |
| 18:CR:36:ASN:HD22 | 18:CR:36:ASN:N     | 2.09                     | 0.48              |
| 20:CT:25:ARG:HG3  | 20:CT:25:ARG:HH11  | 1.78                     | 0.48              |
| 23:CW:73:C:C2'    | 23:CW:74:C:H5'     | 2.25                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:D1:18:ILE:HG21 | 50:D1:20:ARG:NH2   | 2.28                     | 0.48              |
| 50:D1:44:PRO:O    | 50:D1:46:LEU:HD22  | 2.13                     | 0.48              |
| 52:D3:7:LYS:NZ    | 52:D3:32:GLN:HE22  | 2.11                     | 0.48              |
| 57:D8:32:LEU:HB3  | 57:D8:36:LYS:HZ3   | 1.78                     | 0.48              |
| 57:D8:53:PRO:O    | 57:D8:56:GLU:HB2   | 2.12                     | 0.48              |
| 57:D8:62:LEU:HB2  | 57:D8:63:PRO:HD3   | 1.94                     | 0.48              |
| 27:DA:106:C:O2'   | 27:DA:107:C:H5'    | 2.12                     | 0.48              |
| 27:DA:1157:G:O2'  | 27:DA:1158:C:H5'   | 2.14                     | 0.48              |
| 27:DA:1247:A:OP1  | 32:DF:95:ARG:NH2   | 2.46                     | 0.48              |
| 27:DA:1366:A:O2'  | 27:DA:1367:A:H5'   | 2.13                     | 0.48              |
| 27:DA:1495:A:H2'  | 27:DA:1496:A:H2    | 1.76                     | 0.48              |
| 27:DA:1764:G:N2   | 27:DA:1765:C:H1'   | 2.29                     | 0.48              |
| 27:DA:1805:U:C5'  | 30:DD:250:TRP:CD2  | 2.96                     | 0.48              |
| 27:DA:1897:G:N2   | 27:DA:1898:U:H1'   | 2.28                     | 0.48              |
| 27:DA:194:G:H2'   | 27:DA:195:A:O4'    | 2.12                     | 0.48              |
| 27:DA:957:A:C6    | 27:DA:2459:A:C8    | 3.02                     | 0.48              |
| 27:DA:336:C:H2'   | 27:DA:337:C:C6     | 2.48                     | 0.48              |
| 27:DA:430:G:H8    | 27:DA:430:G:O5'    | 1.95                     | 0.48              |
| 27:DA:464:U:H4'   | 56:D7:5:TRP:CZ3    | 2.47                     | 0.48              |
| 28:DB:12:C:O2'    | 28:DB:13:A:OP2     | 2.31                     | 0.48              |
| 28:DB:98:G:H2'    | 28:DB:99:G:H8      | 1.76                     | 0.48              |
| 30:DD:134:ARG:HG3 | 30:DD:135:PHE:CE2  | 2.48                     | 0.48              |
| 30:DD:259:THR:O   | 30:DD:259:THR:HG23 | 2.13                     | 0.48              |
| 34:DH:52:VAL:HG12 | 34:DH:53:GLU:O     | 2.14                     | 0.48              |
| 35:DI:38:LEU:HD12 | 35:DI:38:LEU:N     | 2.28                     | 0.48              |
| 27:DA:587:C:C3'   | 38:DP:33:ARG:NH2   | 2.74                     | 0.48              |
| 40:DR:17:ARG:O    | 40:DR:20:LEU:HB3   | 2.13                     | 0.48              |
| 40:DR:28:LEU:HA   | 40:DR:34:ILE:HG13  | 1.95                     | 0.48              |
| 41:DS:43:GLU:O    | 41:DS:44:LYS:HB2   | 2.12                     | 0.48              |
| 43:DU:101:ARG:C   | 43:DU:102:GLU:HG2  | 2.33                     | 0.48              |
| 43:DU:90:VAL:O    | 43:DU:92:ARG:N     | 2.38                     | 0.48              |
| 43:DU:95:LEU:HD12 | 44:DV:11:GLN:HE21  | 1.77                     | 0.48              |
| 1:AA:1019:C:H2'   | 1:AA:1020:U:O4'    | 2.14                     | 0.48              |
| 1:AA:1069:C:H2'   | 1:AA:1070:U:O5'    | 2.14                     | 0.48              |
| 1:AA:1145:C:H5'   | 1:AA:1146:A:OP1    | 2.12                     | 0.48              |
| 1:AA:1246:C:O2'   | 1:AA:1247:U:H5'    | 2.13                     | 0.48              |
| 1:AA:1309:G:O2'   | 13:AM:77:ASN:ND2   | 2.46                     | 0.48              |
| 1:AA:1530:G:O2'   | 1:AA:1531:A:O5'    | 2.27                     | 0.48              |
| 1:AA:18:C:H4'     | 1:AA:1078:U:O2     | 2.13                     | 0.48              |
| 1:AA:243:A:C2     | 1:AA:245:C:C2      | 3.01                     | 0.48              |
| 1:AA:423:G:H2'    | 1:AA:424:G:H5'     | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:817:C:H6      | 1:AA:817:C:O5'     | 1.96                     | 0.48              |
| 1:AA:916:G:H2'     | 1:AA:917:G:H8      | 1.78                     | 0.48              |
| 1:AA:1190:G:H5'    | 3:AC:176:HIS:HE2   | 1.78                     | 0.48              |
| 4:AD:162:LEU:CD1   | 4:AD:181:MET:SD    | 3.02                     | 0.48              |
| 4:AD:57:ARG:O      | 4:AD:206:PHE:HB2   | 2.13                     | 0.48              |
| 5:AE:43:LEU:HD12   | 5:AE:44:GLY:H      | 1.78                     | 0.48              |
| 5:AE:56:GLN:O      | 5:AE:59:GLY:N      | 2.46                     | 0.48              |
| 7:AG:11:GLN:HG3    | 7:AG:12:LEU:N      | 2.29                     | 0.48              |
| 7:AG:69:VAL:HG11   | 7:AG:104:LEU:HD22  | 1.95                     | 0.48              |
| 12:AL:50:ARG:HG2   | 12:AL:50:ARG:NH1   | 2.27                     | 0.48              |
| 14:AN:23:ARG:HH11  | 14:AN:30:ALA:HB2   | 1.79                     | 0.48              |
| 16:AP:7:ALA:O      | 16:AP:9:PHE:CD2    | 2.66                     | 0.48              |
| 19:AS:32:LYS:HB3   | 19:AS:57:HIS:ND1   | 2.28                     | 0.48              |
| 23:AW:74:C:H4'     | 27:BA:2573:C:H42   | 1.77                     | 0.48              |
| 24:AX:2:G:H4'      | 49:B0:7:LEU:O      | 2.13                     | 0.48              |
| 50:B1:3:LYS:HD2    | 50:B1:4:VAL:HG12   | 1.96                     | 0.48              |
| 27:BA:1017:G:H2'   | 27:BA:1018:C:H6    | 1.77                     | 0.48              |
| 27:BA:1344:G:H5'   | 27:BA:1384:A:C6    | 2.48                     | 0.48              |
| 27:BA:141:A:C8     | 27:BA:1408:C:O2'   | 2.59                     | 0.48              |
| 27:BA:1476:C:H2'   | 27:BA:1477:A:C8    | 2.45                     | 0.48              |
| 27:BA:1846:G:N2    | 27:BA:1895:C:C2    | 2.81                     | 0.48              |
| 27:BA:2594:C:H2'   | 27:BA:2595:G:H8    | 1.76                     | 0.48              |
| 27:BA:271(T):C:H2' | 27:BA:271(U):G:H8  | 1.78                     | 0.48              |
| 27:BA:2783:G:C6    | 27:BA:2784:C:C4    | 3.02                     | 0.48              |
| 27:BA:2834:G:H8    | 27:BA:2834:G:H5''  | 1.79                     | 0.48              |
| 27:BA:2879:C:C4'   | 27:BA:2880:C:OP1   | 2.53                     | 0.48              |
| 27:BA:336:C:H2'    | 27:BA:337:C:C6     | 2.48                     | 0.48              |
| 27:BA:681:G:C4     | 27:BA:682:G:C8     | 3.02                     | 0.48              |
| 27:BA:759:G:C2     | 27:BA:760:G:C8     | 3.02                     | 0.48              |
| 27:BA:951:C:C4     | 27:BA:952:G:N7     | 2.81                     | 0.48              |
| 29:BC:58:VAL:HG21  | 29:BC:166:ASP:N    | 2.28                     | 0.48              |
| 31:BE:86:PRO:O     | 31:BE:88:GLY:N     | 2.33                     | 0.48              |
| 32:BF:125:LEU:HD21 | 32:BF:199:TRP:CD2  | 2.48                     | 0.48              |
| 33:BG:18:GLU:HB3   | 33:BG:175:LEU:HD21 | 1.94                     | 0.48              |
| 34:BH:16:SER:HB2   | 34:BH:27:LYS:HB2   | 1.94                     | 0.48              |
| 35:BI:28:ASN:N     | 35:BI:28:ASN:ND2   | 2.61                     | 0.48              |
| 35:BI:29:TYR:HD1   | 35:BI:33:ARG:HE    | 1.61                     | 0.48              |
| 36:BN:131:GLN:HE22 | 36:BN:134:ARG:HD2  | 1.78                     | 0.48              |
| 37:BO:60:ALA:HA    | 37:BO:87:ILE:HG12  | 1.96                     | 0.48              |
| 41:BS:101:LEU:HD22 | 41:BS:101:LEU:C    | 2.34                     | 0.48              |
| 42:BT:28:VAL:O     | 42:BT:29:ARG:HB2   | 2.12                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:BT:72:VAL:HG12  | 42:BT:73:GLU:N    | 2.27                     | 0.48              |
| 45:BW:85:VAL:CG1   | 45:BW:86:LEU:H    | 2.25                     | 0.48              |
| 47:BY:101:LYS:HG2  | 47:BY:102:CYS:N   | 2.29                     | 0.48              |
| 47:BY:43:ASN:C     | 47:BY:44:ILE:HG13 | 2.34                     | 0.48              |
| 48:BZ:116:LEU:HG   | 48:BZ:172:ALA:O   | 2.12                     | 0.48              |
| 48:BZ:76:ASP:OD2   | 48:BZ:78:ARG:O    | 2.31                     | 0.48              |
| 1:CA:1013:G:H2'    | 1:CA:1015:A:OP2   | 2.13                     | 0.48              |
| 1:CA:1293:G:O2'    | 1:CA:1294:G:H5'   | 2.14                     | 0.48              |
| 1:CA:130:A:H1'     | 1:CA:263:A:O2'    | 2.13                     | 0.48              |
| 1:CA:1329:A:H4'    | 13:CM:24:GLY:O    | 2.13                     | 0.48              |
| 1:CA:338:A:N6      | 1:CA:351:G:H1     | 2.12                     | 0.48              |
| 1:CA:407:G:H2'     | 1:CA:408:A:C8     | 2.41                     | 0.48              |
| 1:CA:409:G:OP1     | 4:CD:23:GLY:O     | 2.31                     | 0.48              |
| 1:CA:559:A:H1'     | 1:CA:561:U:H2'    | 1.95                     | 0.48              |
| 2:CB:69:LEU:O      | 2:CB:162:ILE:HA   | 2.13                     | 0.48              |
| 3:CC:184:TYR:HD1   | 3:CC:201:TYR:CE2  | 2.31                     | 0.48              |
| 3:CC:51:GLY:O      | 3:CC:70:VAL:HG13  | 2.13                     | 0.48              |
| 8:CH:39:LEU:CD2    | 8:CH:39:LEU:H     | 2.22                     | 0.48              |
| 11:CK:125:PHE:N    | 11:CK:125:PHE:HD1 | 2.11                     | 0.48              |
| 17:CQ:4:LYS:HE3    | 17:CQ:6:LEU:CD1   | 2.39                     | 0.48              |
| 17:CQ:82:MET:HA    | 17:CQ:85:VAL:CG2  | 2.42                     | 0.48              |
| 18:CR:25:THR:C     | 18:CR:26:LEU:HD23 | 2.34                     | 0.48              |
| 51:D2:52:ASP:O     | 51:D2:53:LEU:C    | 2.52                     | 0.48              |
| 54:D5:16:ARG:HG2   | 54:D5:16:ARG:HH11 | 1.78                     | 0.48              |
| 57:D8:6:THR:HG22   | 57:D8:63:PRO:HG3  | 1.95                     | 0.48              |
| 27:DA:1170:G:H1    | 27:DA:1179:C:H42  | 1.61                     | 0.48              |
| 27:DA:2192:G:C3'   | 27:DA:2193:G:H5'' | 2.42                     | 0.48              |
| 27:DA:2371:G:O2'   | 55:D6:46:HIS:ND1  | 2.46                     | 0.48              |
| 27:DA:267:C:C2     | 27:DA:268:C:C5    | 3.01                     | 0.48              |
| 27:DA:271(D):G:H2' | 27:DA:271(E):U:C6 | 2.48                     | 0.48              |
| 27:DA:704:G:C1'    | 27:DA:727:A:N6    | 2.76                     | 0.48              |
| 27:DA:704:G:HO2'   | 27:DA:705:A:P     | 2.36                     | 0.48              |
| 27:DA:831:G:H5''   | 27:DA:831:G:C8    | 2.49                     | 0.48              |
| 27:DA:876:C:C2'    | 27:DA:877:U:H5'   | 2.43                     | 0.48              |
| 31:DE:52:LEU:HA    | 31:DE:52:LEU:HD12 | 1.73                     | 0.48              |
| 33:DG:96:ARG:O     | 33:DG:99:MET:HB3  | 2.13                     | 0.48              |
| 36:DN:46:VAL:O     | 36:DN:47:ALA:CB   | 2.55                     | 0.48              |
| 27:DA:833:U:H5''   | 38:DP:48:PRO:HB3  | 1.94                     | 0.48              |
| 39:DQ:1:MET:HE3    | 39:DQ:1:MET:O     | 2.13                     | 0.48              |
| 39:DQ:81:VAL:CG2   | 39:DQ:82:ARG:H    | 2.27                     | 0.48              |
| 42:DT:19:LEU:HA    | 42:DT:20:PRO:HD3  | 1.69                     | 0.48              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 42:DT:80:SER:OG  | 42:DT:81:PRO:HD2   | 2.13                     | 0.48              |
| 43:DU:47:TYR:HA  | 43:DU:50:ARG:CZ    | 2.43                     | 0.48              |
| 27:DA:2012:G:C4' | 45:DW:96:ILE:HD11  | 2.43                     | 0.48              |
| 1:AA:1173:G:C4   | 1:AA:1174:G:C8     | 3.01                     | 0.48              |
| 1:AA:1381:U:C5   | 7:AG:156:TRP:HZ3   | 2.31                     | 0.48              |
| 1:AA:142:G:N3    | 1:AA:142:G:H2'     | 2.29                     | 0.48              |
| 1:AA:372:C:N4    | 1:AA:389:A:H62     | 2.11                     | 0.48              |
| 1:AA:486:U:O2'   | 1:AA:487:A:O5'     | 2.31                     | 0.48              |
| 2:AB:171:ALA:O   | 2:AB:172:ILE:C     | 2.51                     | 0.48              |
| 2:AB:197:VAL:CB  | 2:AB:200:ILE:HG12  | 2.42                     | 0.48              |
| 4:AD:152:SER:C   | 4:AD:154:ASN:N     | 2.66                     | 0.48              |
| 9:AI:11:LYS:C    | 9:AI:13:ALA:H      | 2.16                     | 0.48              |
| 9:AI:53:VAL:CG2  | 9:AI:54:ASP:N      | 2.54                     | 0.48              |
| 11:AK:33:THR:HA  | 11:AK:39:PRO:HA    | 1.95                     | 0.48              |
| 11:AK:66:LEU:O   | 11:AK:69:ALA:N     | 2.45                     | 0.48              |
| 13:AM:102:ARG:CG | 13:AM:102:ARG:HH11 | 2.27                     | 0.48              |
| 15:AO:77:ARG:O   | 15:AO:81:LEU:HB3   | 2.13                     | 0.48              |
| 18:AR:87:ARG:HG2 | 18:AR:87:ARG:NH1   | 2.28                     | 0.48              |
| 1:AA:1313:U:O4   | 19:AS:4:SER:N      | 2.47                     | 0.48              |
| 20:AT:60:GLU:HG3 | 20:AT:81:LYS:HE3   | 1.95                     | 0.48              |
| 23:AW:30:A:H2'   | 23:AW:31:U:C5'     | 2.26                     | 0.48              |
| 27:BA:464:U:H4'  | 56:B7:5:TRP:CH2    | 2.48                     | 0.48              |
| 27:BA:1001:A:H2' | 27:BA:1002:G:O4'   | 2.13                     | 0.48              |
| 27:BA:2031:A:C6  | 27:BA:2498:C:H1'   | 2.48                     | 0.48              |
| 27:BA:2346:A:C8  | 27:BA:2383:G:C6    | 3.01                     | 0.48              |
| 27:BA:2536:G:C6  | 27:BA:2537:U:C4    | 3.02                     | 0.48              |
| 27:BA:27:G:O2'   | 27:BA:28:A:P       | 2.72                     | 0.48              |
| 27:BA:535:C:C2'  | 27:BA:536:A:H5'    | 2.43                     | 0.48              |
| 27:BA:558:G:OP1  | 36:BN:111:PRO:HD2  | 2.13                     | 0.48              |
| 27:BA:696:G:H2'  | 27:BA:697:C:H6     | 1.79                     | 0.48              |
| 27:BA:68:G:N2    | 27:BA:74:A:C4      | 2.81                     | 0.48              |
| 27:BA:764:A:C5   | 30:BD:209:ALA:HB3  | 2.49                     | 0.48              |
| 27:BA:785:G:N3   | 27:BA:785:G:H2'    | 2.27                     | 0.48              |
| 27:BA:875:G:C6   | 27:BA:876:C:C2     | 3.02                     | 0.48              |
| 28:BB:42:C:H2'   | 28:BB:43:C:H6      | 1.78                     | 0.48              |
| 28:BB:45:A:C2'   | 28:BB:46:A:H5'     | 2.43                     | 0.48              |
| 30:BD:130:ALA:C  | 30:BD:131:LEU:HD12 | 2.33                     | 0.48              |
| 30:BD:238:GLY:O  | 30:BD:239:ARG:O    | 2.31                     | 0.48              |
| 30:BD:72:LYS:HG3 | 30:BD:97:TYR:CE2   | 2.48                     | 0.48              |
| 33:BG:56:ALA:O   | 33:BG:60:LEU:HB2   | 2.13                     | 0.48              |
| 34:BH:137:ASP:O  | 34:BH:138:LYS:CB   | 2.61                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BH:29:PRO:O    | 34:BH:30:LYS:CE    | 2.60                     | 0.48              |
| 34:BH:61:HIS:O    | 34:BH:62:LYS:C     | 2.52                     | 0.48              |
| 36:BN:70:LYS:HB3  | 36:BN:87:LEU:HD12  | 1.95                     | 0.48              |
| 38:BP:16:ARG:HG3  | 38:BP:17:LYS:N     | 2.28                     | 0.48              |
| 38:BP:50:ARG:HB3  | 57:B8:59:LYS:CD    | 2.37                     | 0.48              |
| 39:BQ:57:HIS:HE1  | 39:BQ:116:GLU:CG   | 2.25                     | 0.48              |
| 39:BQ:118:LEU:O   | 39:BQ:119:ARG:C    | 2.52                     | 0.48              |
| 44:BV:13:ARG:NH1  | 44:BV:13:ARG:HG2   | 2.23                     | 0.48              |
| 44:BV:49:THR:HG22 | 44:BV:50:PRO:CD    | 2.39                     | 0.48              |
| 47:BY:14:LEU:HD12 | 47:BY:15:VAL:N     | 2.28                     | 0.48              |
| 48:BZ:152:SER:N   | 48:BZ:166:PRO:HB3  | 2.24                     | 0.48              |
| 1:CA:1113:C:H6    | 1:CA:1113:C:O5'    | 1.96                     | 0.48              |
| 1:CA:1157:A:C4'   | 1:CA:1158:C:O5'    | 2.54                     | 0.48              |
| 1:CA:1053:G:N7    | 1:CA:1199:U:H2'    | 2.28                     | 0.48              |
| 1:CA:985:C:N3     | 1:CA:1221:G:C2     | 2.82                     | 0.48              |
| 1:CA:1326:C:H2'   | 1:CA:1327:C:C6     | 2.49                     | 0.48              |
| 1:CA:344:A:H3'    | 1:CA:346:G:O6      | 2.13                     | 0.48              |
| 1:CA:613:C:H2'    | 1:CA:614:A:C8      | 2.45                     | 0.48              |
| 3:CC:206:GLU:O    | 3:CC:207:VAL:C     | 2.51                     | 0.48              |
| 4:CD:92:VAL:O     | 4:CD:93:PHE:C      | 2.52                     | 0.48              |
| 6:CF:42:GLU:O     | 6:CF:44:GLY:N      | 2.46                     | 0.48              |
| 11:CK:33:THR:HB   | 11:CK:37:GLY:O     | 2.12                     | 0.48              |
| 12:CL:98:VAL:HG12 | 12:CL:101:VAL:CG2  | 2.43                     | 0.48              |
| 15:CO:62:GLN:O    | 15:CO:66:LEU:HD22  | 2.14                     | 0.48              |
| 20:CT:67:ALA:HA   | 20:CT:73:HIS:HA    | 1.95                     | 0.48              |
| 55:D6:11:LEU:O    | 55:D6:24:GLU:N     | 2.47                     | 0.48              |
| 27:DA:1764:G:N2   | 27:DA:1765:C:C2    | 2.81                     | 0.48              |
| 27:DA:1893:C:H2'  | 27:DA:1894:C:O5'   | 2.13                     | 0.48              |
| 27:DA:1916:A:H2'  | 27:DA:1917:U:O4'   | 2.14                     | 0.48              |
| 27:DA:2122:U:H2'  | 27:DA:2123:G:H8    | 1.77                     | 0.48              |
| 27:DA:2206:G:N3   | 27:DA:2206:G:H5''  | 2.29                     | 0.48              |
| 27:DA:2318:G:C2'  | 27:DA:2319:G:OP1   | 2.60                     | 0.48              |
| 27:DA:2440:C:H2'  | 27:DA:2441:C:O5'   | 2.13                     | 0.48              |
| 27:DA:2562:U:O2   | 27:DA:2562:U:C2'   | 2.52                     | 0.48              |
| 27:DA:271(A):A:N1 | 27:DA:272(D):G:O2' | 2.46                     | 0.48              |
| 27:DA:448:U:H3'   | 27:DA:449:A:C5'    | 2.42                     | 0.48              |
| 27:DA:481:G:H1'   | 27:DA:506:G:N2     | 2.25                     | 0.48              |
| 27:DA:536:A:H2'   | 27:DA:537:C:H6     | 1.75                     | 0.48              |
| 27:DA:805:G:H22   | 27:DA:828:U:H5''   | 1.78                     | 0.48              |
| 29:DC:82:LYS:C    | 29:DC:83:ILE:HD13  | 2.34                     | 0.48              |
| 30:DD:58:HIS:C    | 30:DD:58:HIS:CD2   | 2.86                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DE:111:ARG:CD   | 31:DE:160:TYR:CE1 | 2.91                     | 0.48              |
| 32:DF:18:ARG:HG3   | 32:DF:19:GLU:N    | 2.29                     | 0.48              |
| 35:DI:81:VAL:HG11  | 35:DI:88:ILE:HG21 | 1.96                     | 0.48              |
| 37:DO:23:ARG:HD2   | 37:DO:24:VAL:N    | 2.27                     | 0.48              |
| 38:DP:100:LEU:O    | 38:DP:103:ALA:HB3 | 2.14                     | 0.48              |
| 39:DQ:2:LEU:HG     | 39:DQ:70:PRO:HG3  | 1.96                     | 0.48              |
| 39:DQ:98:LYS:HB3   | 39:DQ:99:PRO:HD2  | 1.94                     | 0.48              |
| 40:DR:9:LYS:O      | 40:DR:10:LEU:HG   | 2.14                     | 0.48              |
| 41:DS:36:TYR:HD1   | 41:DS:36:TYR:N    | 2.11                     | 0.48              |
| 42:DT:73:GLU:OE1   | 42:DT:103:ARG:NE  | 2.47                     | 0.48              |
| 27:DA:2020:A:OP1   | 43:DU:27:LEU:HG   | 2.12                     | 0.48              |
| 45:DW:55:ALA:O     | 45:DW:57:ASN:N    | 2.37                     | 0.48              |
| 48:DZ:8:TYR:HE1    | 48:DZ:62:ASP:OD2  | 1.95                     | 0.48              |
| 1:AA:115:G:H4'     | 1:AA:116:A:O5'    | 2.13                     | 0.48              |
| 1:AA:1278:U:C3'    | 1:AA:1278:U:C6    | 2.95                     | 0.48              |
| 1:AA:148:G:H2'     | 1:AA:149:A:C8     | 2.48                     | 0.48              |
| 1:AA:924:C:O2'     | 1:AA:1502:A:N6    | 2.47                     | 0.48              |
| 1:AA:191:G:O2'     | 1:AA:192:U:H5'    | 2.14                     | 0.48              |
| 1:AA:372:C:H42     | 1:AA:389:A:N6     | 2.12                     | 0.48              |
| 1:AA:422:C:O2'     | 1:AA:423:G:OP2    | 2.29                     | 0.48              |
| 2:AB:102:LEU:H     | 2:AB:102:LEU:HD12 | 1.78                     | 0.48              |
| 2:AB:39:ILE:O      | 2:AB:41:ILE:HD12  | 2.14                     | 0.48              |
| 3:AC:175:LEU:H     | 3:AC:175:LEU:HD12 | 1.77                     | 0.48              |
| 1:AA:437:U:O2'     | 4:AD:123:HIS:HD2  | 1.96                     | 0.48              |
| 4:AD:161:ASN:OD1   | 4:AD:161:ASN:N    | 2.46                     | 0.48              |
| 7:AG:108:ALA:O     | 7:AG:111:ARG:HB2  | 2.13                     | 0.48              |
| 7:AG:73:MET:HA     | 7:AG:91:VAL:HG23  | 1.96                     | 0.48              |
| 8:AH:42:GLU:HG3    | 8:AH:109:ILE:HD12 | 1.96                     | 0.48              |
| 8:AH:109:ILE:HG12  | 8:AH:110:ALA:N    | 2.28                     | 0.48              |
| 11:AK:116:HIS:ND1  | 11:AK:116:HIS:N   | 2.61                     | 0.48              |
| 11:AK:126:ARG:HH11 | 11:AK:126:ARG:HB3 | 1.78                     | 0.48              |
| 1:AA:706:A:H5''    | 11:AK:22:HIS:CD2  | 2.49                     | 0.48              |
| 12:AL:112:LYS:C    | 12:AL:114:ARG:H   | 2.17                     | 0.48              |
| 12:AL:76:GLU:O     | 12:AL:77:HIS:CB   | 2.55                     | 0.48              |
| 13:AM:13:LYS:C     | 13:AM:44:ARG:HD2  | 2.34                     | 0.48              |
| 20:AT:100:ILE:O    | 20:AT:102:GLY:N   | 2.47                     | 0.48              |
| 51:B2:47:ASN:O     | 51:B2:50:ILE:N    | 2.41                     | 0.48              |
| 27:BA:1943:U:C1'   | 27:BA:1945:G:H5'  | 2.43                     | 0.48              |
| 27:BA:1971:A:C5    | 30:BD:241:PRO:HG3 | 2.48                     | 0.48              |
| 27:BA:2355:C:H1'   | 49:B0:39:ARG:NH2  | 2.21                     | 0.48              |
| 27:BA:2631:G:H1    | 27:BA:2787:C:H42  | 1.62                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:286:C:O2'   | 27:BA:287:C:C5'    | 2.61                     | 0.48              |
| 27:BA:355:G:C4    | 27:BA:356:G:C8     | 3.02                     | 0.48              |
| 27:BA:358:U:O2    | 27:BA:358:U:H2'    | 2.12                     | 0.48              |
| 27:BA:388:G:H5'   | 50:B1:25:LYS:HG2   | 1.95                     | 0.48              |
| 27:BA:435:C:O2'   | 27:BA:436:C:H5'    | 2.13                     | 0.48              |
| 27:BA:686:G:O6    | 56:B7:12:ARG:HA    | 2.14                     | 0.48              |
| 27:BA:794:G:C2    | 27:BA:795:C:C2     | 3.01                     | 0.48              |
| 30:BD:118:VAL:N   | 30:BD:129:ASN:OD1  | 2.46                     | 0.48              |
| 34:BH:43:VAL:HG11 | 34:BH:52:VAL:CA    | 2.44                     | 0.48              |
| 34:BH:54:ARG:HG2  | 34:BH:65:HIS:CD2   | 2.45                     | 0.48              |
| 35:BI:107:VAL:O   | 35:BI:109:ILE:HD13 | 2.13                     | 0.48              |
| 35:BI:33:ARG:O    | 35:BI:35:LEU:HD23  | 2.14                     | 0.48              |
| 44:BV:43:GLU:HA   | 44:BV:43:GLU:OE1   | 2.11                     | 0.48              |
| 46:BX:5:TYR:CE1   | 51:B2:30:ARG:HB2   | 2.48                     | 0.48              |
| 48:BZ:75:LEU:HD22 | 48:BZ:82:PRO:HA    | 1.95                     | 0.48              |
| 1:CA:1354:C:H2'   | 1:CA:1355:G:C8     | 2.49                     | 0.48              |
| 1:CA:189(D):C:N3  | 1:CA:189(E):U:C2   | 2.81                     | 0.48              |
| 1:CA:218:C:O2'    | 1:CA:219:C:H6      | 1.97                     | 0.48              |
| 1:CA:260:G:H2'    | 1:CA:261:U:H6      | 1.79                     | 0.48              |
| 1:CA:725:G:H2'    | 1:CA:726:C:H6      | 1.79                     | 0.48              |
| 1:CA:876:G:P      | 8:CH:14:ARG:NH1    | 2.87                     | 0.48              |
| 1:CA:923:A:C6     | 1:CA:924:C:N3      | 2.81                     | 0.48              |
| 1:CA:977:A:C8     | 1:CA:982:U:O4      | 2.67                     | 0.48              |
| 2:CB:178:ARG:NH2  | 8:CH:68:ARG:NH2    | 2.51                     | 0.48              |
| 4:CD:98:GLU:OE2   | 4:CD:103:ASN:ND2   | 2.44                     | 0.48              |
| 6:CF:61:LEU:HD23  | 6:CF:63:TYR:OH     | 2.13                     | 0.48              |
| 6:CF:82:ARG:CB    | 6:CF:85:VAL:HG23   | 2.44                     | 0.48              |
| 8:CH:104:ARG:O    | 8:CH:106:GLY:N     | 2.46                     | 0.48              |
| 9:CI:32:ASP:OD1   | 9:CI:33:PHE:N      | 2.47                     | 0.48              |
| 10:CJ:85:LEU:O    | 10:CJ:87:THR:N     | 2.46                     | 0.48              |
| 10:CJ:94:VAL:CG1  | 10:CJ:95:GLU:H     | 2.25                     | 0.48              |
| 12:CL:99:ARG:NH2  | 12:CL:107:VAL:HG22 | 2.29                     | 0.48              |
| 25:CY:31:U:O2'    | 25:CY:32:U:H5'     | 2.14                     | 0.48              |
| 50:D1:29:GLY:O    | 50:D1:30:VAL:CG2   | 2.62                     | 0.48              |
| 50:D1:12:PRO:HB2  | 50:D1:41:ARG:HD3   | 1.96                     | 0.48              |
| 27:DA:969:U:P     | 52:D3:17:LYS:HG2   | 2.54                     | 0.48              |
| 57:D8:55:ALA:O    | 57:D8:59:LYS:HG3   | 2.13                     | 0.48              |
| 27:DA:1558:A:HO2' | 27:DA:1559:G:P     | 2.37                     | 0.48              |
| 27:DA:1693:U:O2'  | 27:DA:1694:C:OP1   | 2.31                     | 0.48              |
| 27:DA:2765:A:N3   | 27:DA:2765:A:H3'   | 2.28                     | 0.48              |
| 27:DA:345:A:C4'   | 27:DA:346:A:OP1    | 2.60                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:458:G:C8    | 56:D7:37:LYS:NZ   | 2.81                     | 0.48              |
| 27:DA:533:G:H5'   | 43:DU:24:TYR:CD2  | 2.49                     | 0.48              |
| 27:DA:841:A:H2'   | 27:DA:842:G:C8    | 2.49                     | 0.48              |
| 27:DA:869:G:N3    | 27:DA:870:A:C8    | 2.82                     | 0.48              |
| 27:DA:992:C:H3'   | 27:DA:992:C:C6    | 2.48                     | 0.48              |
| 29:DC:77:ILE:HG21 | 29:DC:123:VAL:N   | 2.25                     | 0.48              |
| 30:DD:119:ALA:HB2 | 30:DD:130:ALA:HB3 | 1.96                     | 0.48              |
| 30:DD:142:VAL:CG2 | 30:DD:143:HIS:N   | 2.76                     | 0.48              |
| 30:DD:51:VAL:HG11 | 30:DD:54:ARG:HE   | 1.78                     | 0.48              |
| 34:DH:38:SER:C    | 34:DH:40:GLU:N    | 2.67                     | 0.48              |
| 36:DN:10:GLU:HA   | 36:DN:11:PRO:HD3  | 1.75                     | 0.48              |
| 37:DO:10:VAL:HG22 | 37:DO:10:VAL:O    | 2.14                     | 0.48              |
| 40:DR:2:ARG:NH2   | 40:DR:5:LYS:CE    | 2.77                     | 0.48              |
| 41:DS:21:THR:O    | 41:DS:23:ARG:N    | 2.46                     | 0.48              |
| 41:DS:40:ILE:HG22 | 41:DS:40:ILE:O    | 2.14                     | 0.48              |
| 27:DA:143:G:H1'   | 46:DX:37:THR:CG2  | 2.43                     | 0.48              |
| 1:AA:1033:G:H2'   | 1:AA:1034:G:H5'   | 1.96                     | 0.48              |
| 1:AA:1221:G:H4'   | 19:AS:77:THR:CG2  | 2.44                     | 0.48              |
| 1:AA:1321:C:OP2   | 1:AA:1322:C:H2'   | 2.14                     | 0.48              |
| 1:AA:442:C:H42    | 1:AA:492:G:H1     | 1.62                     | 0.48              |
| 1:AA:505:G:H2'    | 1:AA:506:G:H8     | 1.78                     | 0.48              |
| 2:AB:95:GLN:HA    | 2:AB:95:GLN:OE1   | 2.14                     | 0.48              |
| 3:AC:89:GLU:HG3   | 3:AC:90:GLU:N     | 2.28                     | 0.48              |
| 4:AD:3:ARG:CB     | 4:AD:118:ARG:HH11 | 2.25                     | 0.48              |
| 5:AE:29:GLY:HA2   | 5:AE:46:GLY:O     | 2.14                     | 0.48              |
| 10:AJ:24:VAL:O    | 10:AJ:28:ARG:HB2  | 2.14                     | 0.48              |
| 11:AK:44:SER:H    | 11:AK:47:VAL:CG2  | 2.26                     | 0.48              |
| 1:AA:275:G:H4'    | 17:AQ:14:LYS:O    | 2.13                     | 0.48              |
| 13:AM:88:ARG:HH21 | 19:AS:69:HIS:HE1  | 1.62                     | 0.48              |
| 20:AT:87:LYS:HG3  | 20:AT:91:LEU:CD1  | 2.43                     | 0.48              |
| 24:AX:20:U:H3'    | 24:AX:21:A:H5''   | 1.96                     | 0.48              |
| 50:B1:75:GLU:C    | 50:B1:77:ALA:H    | 2.16                     | 0.48              |
| 27:BA:1303:G:H1'  | 27:BA:1641:A:N1   | 2.29                     | 0.48              |
| 27:BA:1675:C:O2   | 31:BE:129:HIS:N   | 2.46                     | 0.48              |
| 27:BA:1846:G:C5'  | 27:BA:1847:A:OP2  | 2.62                     | 0.48              |
| 27:BA:1980:G:H4'  | 27:BA:1981:A:OP2  | 2.13                     | 0.48              |
| 27:BA:185:U:H4'   | 27:BA:218:A:H4'   | 1.96                     | 0.48              |
| 27:BA:232:G:C4'   | 27:BA:233:A:OP1   | 2.53                     | 0.48              |
| 27:BA:2534:A:H5'  | 27:BA:2534:A:H8   | 1.79                     | 0.48              |
| 27:BA:2553:G:H2'  | 27:BA:2554:U:O4'  | 2.13                     | 0.48              |
| 27:BA:2594:C:O2'  | 27:BA:2595:G:H5'  | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:2600:A:H2'   | 27:BA:2601:C:C6    | 2.49                     | 0.48              |
| 27:BA:2615:U:C2    | 54:B5:7:PRO:HA     | 2.49                     | 0.48              |
| 27:BA:2706:G:H8    | 27:BA:2706:G:O5'   | 1.96                     | 0.48              |
| 27:BA:271(D):G:O2' | 27:BA:271(E):U:H5' | 2.14                     | 0.48              |
| 27:BA:2832:U:O2    | 27:BA:2834:G:N1    | 2.46                     | 0.48              |
| 27:BA:826:U:H5''   | 27:BA:826:U:C6     | 2.47                     | 0.48              |
| 29:BC:49:ILE:HD12  | 29:BC:49:ILE:N     | 2.21                     | 0.48              |
| 30:BD:70:TRP:CH2   | 30:BD:150:LYS:HA   | 2.48                     | 0.48              |
| 32:BF:167:ALA:O    | 32:BF:169:ASN:N    | 2.47                     | 0.48              |
| 35:BI:79:ILE:HG23  | 35:BI:80:PRO:HD2   | 1.95                     | 0.48              |
| 36:BN:31:ALA:O     | 36:BN:34:LEU:HB2   | 2.13                     | 0.48              |
| 38:BP:65:ARG:NH2   | 57:B8:15:LYS:HD2   | 2.29                     | 0.48              |
| 39:BQ:27:VAL:HG23  | 39:BQ:137:TYR:HE1  | 1.78                     | 0.48              |
| 40:BR:101:ALA:HB2  | 54:B5:44:THR:CB    | 2.43                     | 0.48              |
| 40:BR:24:GLN:O     | 40:BR:25:ALA:C     | 2.51                     | 0.48              |
| 41:BS:67:ARG:NH2   | 41:BS:100:ALA:HB3  | 2.28                     | 0.48              |
| 42:BT:28:VAL:HG22  | 42:BT:46:GLU:C     | 2.34                     | 0.48              |
| 42:BT:65:LYS:NZ    | 42:BT:66:VAL:N     | 2.62                     | 0.48              |
| 43:BU:92:ARG:HE    | 43:BU:95:LEU:HD12  | 1.78                     | 0.48              |
| 44:BV:36:PRO:HA    | 44:BV:56:SER:HA    | 1.95                     | 0.48              |
| 27:BA:2010:G:H5'   | 45:BW:42:ARG:HB2   | 1.95                     | 0.48              |
| 1:CA:1096:C:C2     | 1:CA:1097:C:C5     | 3.02                     | 0.48              |
| 1:CA:173:U:H1'     | 1:CA:197:A:C6      | 2.49                     | 0.48              |
| 1:CA:189(E):U:O2'  | 1:CA:189(F):U:H5'' | 2.13                     | 0.48              |
| 1:CA:317:G:H2'     | 1:CA:318:G:C8      | 2.49                     | 0.48              |
| 1:CA:375:U:H2'     | 1:CA:376:G:H8      | 1.79                     | 0.48              |
| 1:CA:434:U:H2'     | 1:CA:435:C:C6      | 2.48                     | 0.48              |
| 1:CA:540:G:H2'     | 1:CA:541:G:H8      | 1.79                     | 0.48              |
| 1:CA:647:C:C4      | 1:CA:648:A:N7      | 2.81                     | 0.48              |
| 1:CA:651:C:N4      | 1:CA:753:A:OP2     | 2.40                     | 0.48              |
| 1:CA:960:U:O2'     | 1:CA:1223:C:H5'    | 2.13                     | 0.48              |
| 1:CA:982:U:OP1     | 1:CA:982:U:H6      | 1.97                     | 0.48              |
| 2:CB:131:PRO:HG2   | 2:CB:134:GLU:CB    | 2.44                     | 0.48              |
| 2:CB:174:VAL:O     | 2:CB:174:VAL:HG12  | 2.14                     | 0.48              |
| 2:CB:189:ASP:OD2   | 2:CB:191:ASP:HB2   | 2.14                     | 0.48              |
| 4:CD:9:CYS:SG      | 4:CD:12:CYS:SG     | 3.11                     | 0.48              |
| 4:CD:15:GLU:OE1    | 4:CD:15:GLU:N      | 2.46                     | 0.48              |
| 8:CH:73:ASP:OD2    | 8:CH:73:ASP:C      | 2.52                     | 0.48              |
| 9:CI:19:LEU:HD23   | 9:CI:61:ALA:HB2    | 1.95                     | 0.48              |
| 9:CI:27:THR:HG23   | 9:CI:31:GLN:O      | 2.14                     | 0.48              |
| 13:CM:29:ARG:HD3   | 13:CM:64:TRP:CZ3   | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:CM:37:THR:OG1  | 13:CM:39:ILE:HG13 | 2.14                     | 0.48              |
| 16:CP:31:LYS:CG   | 16:CP:32:TYR:H    | 2.24                     | 0.48              |
| 1:CA:473:G:H5''   | 16:CP:81:ARG:HE   | 1.77                     | 0.48              |
| 1:CA:790:A:OP1    | 24:CX:38:A:O2'    | 2.31                     | 0.48              |
| 25:CY:68:C:H2'    | 25:CY:69:C:C5'    | 2.36                     | 0.48              |
| 27:DA:851:U:O2'   | 52:D3:45:GLY:HA3  | 2.14                     | 0.48              |
| 52:D3:59:VAL:CG1  | 52:D3:60:GLU:N    | 2.66                     | 0.48              |
| 27:DA:1019:U:O2'  | 27:DA:1021:A:C2   | 2.55                     | 0.48              |
| 27:DA:1644:C:O2   | 27:DA:1644:C:H2'  | 2.11                     | 0.48              |
| 27:DA:2247:A:C5   | 27:DA:2248:C:C5   | 3.02                     | 0.48              |
| 27:DA:2347:C:H2'  | 27:DA:2348:U:C6   | 2.48                     | 0.48              |
| 27:DA:2367:G:H2'  | 27:DA:2368:C:C6   | 2.47                     | 0.48              |
| 27:DA:2539:C:C2   | 27:DA:2540:C:C5   | 3.02                     | 0.48              |
| 27:DA:1953:A:H2   | 27:DA:2549:G:N3   | 2.12                     | 0.48              |
| 27:DA:2571:C:H5'' | 27:DA:2572:A:C5'  | 2.44                     | 0.48              |
| 27:DA:304:G:H2'   | 27:DA:305:U:C6    | 2.49                     | 0.48              |
| 27:DA:425:G:O2'   | 27:DA:426:C:H5'   | 2.13                     | 0.48              |
| 27:DA:475:U:C5    | 27:DA:481:G:O6    | 2.66                     | 0.48              |
| 27:DA:682:G:O2'   | 27:DA:683:C:H5'   | 2.13                     | 0.48              |
| 27:DA:704:G:O2'   | 27:DA:705:A:P     | 2.71                     | 0.48              |
| 27:DA:669:G:C2    | 27:DA:801:G:C6    | 3.02                     | 0.48              |
| 27:DA:858:U:C2    | 27:DA:920:G:N2    | 2.82                     | 0.48              |
| 27:DA:952:G:N1    | 27:DA:966:G:C6    | 2.82                     | 0.48              |
| 30:DD:102:LYS:C   | 30:DD:103:ARG:HG2 | 2.34                     | 0.48              |
| 30:DD:176:ARG:HD2 | 30:DD:180:GLY:HA2 | 1.94                     | 0.48              |
| 31:DE:200:GLU:N   | 31:DE:200:GLU:OE2 | 2.46                     | 0.48              |
| 27:DA:674:G:C1'   | 32:DF:74:ARG:HD3  | 2.44                     | 0.48              |
| 33:DG:2:PRO:O     | 33:DG:3:LEU:CB    | 2.62                     | 0.48              |
| 35:DI:78:THR:CG2  | 35:DI:143:SER:HB2 | 2.42                     | 0.48              |
| 38:DP:138:LEU:O   | 38:DP:139:LYS:C   | 2.51                     | 0.48              |
| 38:DP:39:LYS:O    | 38:DP:41:ARG:HG2  | 2.13                     | 0.48              |
| 27:DA:870:A:H5''  | 39:DQ:6:ARG:O     | 2.14                     | 0.48              |
| 44:DV:40:LEU:CD1  | 44:DV:46:VAL:HA   | 2.42                     | 0.48              |
| 45:DW:12:ILE:HD13 | 45:DW:17:VAL:CG1  | 2.43                     | 0.48              |
| 48:DZ:151:ALA:HB3 | 48:DZ:153:ASP:OD2 | 2.14                     | 0.48              |
| 48:DZ:174:VAL:HB  | 48:DZ:175:PRO:HD2 | 1.95                     | 0.48              |
| 1:AA:1508:G:C5    | 1:AA:1509:C:C5    | 3.01                     | 0.48              |
| 1:AA:35:G:C2'     | 1:AA:36:C:H5'     | 2.43                     | 0.48              |
| 1:AA:736:C:N4     | 1:AA:737:A:H62    | 2.12                     | 0.48              |
| 1:AA:878:G:H8     | 1:AA:878:G:O5'    | 1.96                     | 0.48              |
| 1:AA:960:U:C4     | 1:AA:1225:A:C4    | 3.00                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:AB:112:VAL:O      | 2:AB:115:LEU:HB3    | 2.13                     | 0.48              |
| 2:AB:15:VAL:N       | 2:AB:16:HIS:CE1     | 2.82                     | 0.48              |
| 2:AB:214:ILE:HG22   | 2:AB:215:LEU:N      | 2.28                     | 0.48              |
| 3:AC:202:ILE:O      | 3:AC:204:LEU:HG     | 2.13                     | 0.48              |
| 4:AD:123:HIS:O      | 4:AD:124:GLY:C      | 2.52                     | 0.48              |
| 4:AD:12:CYS:HA      | 4:AD:19:LEU:HB2     | 1.96                     | 0.48              |
| 4:AD:154:ASN:HA     | 4:AD:159:ARG:NH2    | 2.28                     | 0.48              |
| 4:AD:4:TYR:CG       | 4:AD:5:ILE:N        | 2.80                     | 0.48              |
| 4:AD:9:CYS:HA       | 4:AD:12:CYS:HB2     | 1.96                     | 0.48              |
| 1:AA:922:G:H1'      | 5:AE:19:MET:HB3     | 1.95                     | 0.48              |
| 8:AH:17:THR:HG22    | 8:AH:65:TYR:CZ      | 2.49                     | 0.48              |
| 1:AA:963:G:H21      | 10:AJ:55:LYS:HZ3    | 1.60                     | 0.48              |
| 12:AL:83:ARG:HB2    | 12:AL:98:VAL:HG22   | 1.95                     | 0.48              |
| 13:AM:9:ILE:HD12    | 13:AM:9:ILE:N       | 2.29                     | 0.48              |
| 20:AT:26:ASN:CB     | 20:AT:71:THR:HG23   | 2.44                     | 0.48              |
| 20:AT:54:LYS:HA     | 20:AT:57:ARG:NH1    | 2.28                     | 0.48              |
| 49:B0:50:ASN:C      | 49:B0:62:LEU:HD12   | 2.34                     | 0.48              |
| 50:B1:47:GLN:N      | 50:B1:62:VAL:O      | 2.42                     | 0.48              |
| 27:BA:242:G:O5'     | 57:B8:62:LEU:HD22   | 2.14                     | 0.48              |
| 27:BA:1450:G:H2'    | 27:BA:1450(A):C:O5' | 2.14                     | 0.48              |
| 27:BA:1500:G:C2'    | 27:BA:1501:C:O5'    | 2.62                     | 0.48              |
| 27:BA:1668:A:N7     | 27:BA:1674:G:C6     | 2.81                     | 0.48              |
| 27:BA:1721:G:O6     | 27:BA:1739:U:H5'    | 2.14                     | 0.48              |
| 27:BA:1747(A):G:H2' | 27:BA:1748:G:C5'    | 2.17                     | 0.48              |
| 27:BA:1761:C:H3'    | 27:BA:1762:A:C8     | 2.49                     | 0.48              |
| 27:BA:1987:G:C2     | 27:BA:1988:C:C4     | 3.01                     | 0.48              |
| 27:BA:269:U:C5      | 27:BA:271(Y):U:C4   | 3.02                     | 0.48              |
| 27:BA:2746:U:H2'    | 27:BA:2747:G:H5'    | 1.95                     | 0.48              |
| 27:BA:38:A:C2       | 27:BA:442:G:C2      | 3.02                     | 0.48              |
| 27:BA:54:G:OP2      | 27:BA:54:G:H8       | 1.97                     | 0.48              |
| 27:BA:709:U:O2'     | 27:BA:710:G:H5'     | 2.13                     | 0.48              |
| 27:BA:807:U:H2'     | 27:BA:808:G:O4'     | 2.13                     | 0.48              |
| 29:BC:187:ASP:O     | 29:BC:189:ILE:N     | 2.47                     | 0.48              |
| 30:BD:72:LYS:NZ     | 30:BD:103:ARG:HH12  | 2.11                     | 0.48              |
| 30:BD:109:ASP:HB2   | 30:BD:197:GLY:CA    | 2.43                     | 0.48              |
| 30:BD:35:LYS:O      | 30:BD:64:ILE:N      | 2.43                     | 0.48              |
| 32:BF:202:PHE:HA    | 32:BF:205:ARG:HB2   | 1.95                     | 0.48              |
| 34:BH:159:GLU:OE1   | 34:BH:159:GLU:CA    | 2.57                     | 0.48              |
| 35:BI:111:PRO:HA    | 35:BI:114:LEU:CD2   | 2.34                     | 0.48              |
| 35:BI:128:LEU:O     | 35:BI:137:PRO:HA    | 2.13                     | 0.48              |
| 36:BN:35:ARG:HB3    | 36:BN:42:TRP:CH2    | 2.49                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BN:48:MET:H    | 36:BN:48:MET:HE2  | 1.77                     | 0.48              |
| 36:BN:3:THR:HG22  | 36:BN:5:VAL:H     | 1.78                     | 0.48              |
| 37:BO:35:VAL:CG2  | 37:BO:65:THR:HG23 | 2.44                     | 0.48              |
| 38:BP:79:ARG:O    | 38:BP:111:ARG:HB2 | 2.12                     | 0.48              |
| 39:BQ:12:GLN:NE2  | 39:BQ:73:PRO:HD3  | 2.29                     | 0.48              |
| 27:BA:2838:G:H1'  | 40:BR:45:ARG:NH1  | 2.28                     | 0.48              |
| 41:BS:92:TYR:HD1  | 41:BS:92:TYR:N    | 2.10                     | 0.48              |
| 42:BT:55:ASN:C    | 42:BT:59:THR:HG22 | 2.34                     | 0.48              |
| 44:BV:18:LEU:O    | 44:BV:19:LYS:O    | 2.31                     | 0.48              |
| 44:BV:34:GLU:OE2  | 44:BV:56:SER:HB2  | 2.13                     | 0.48              |
| 48:BZ:134:GLU:O   | 48:BZ:135:PHE:HB3 | 2.12                     | 0.48              |
| 1:CA:1104:G:C2'   | 1:CA:1105:A:H5'   | 2.43                     | 0.48              |
| 1:CA:1306:A:N6    | 1:CA:1331:G:H1'   | 2.29                     | 0.48              |
| 1:CA:1325:C:O3'   | 21:CU:17:THR:HG21 | 2.14                     | 0.48              |
| 1:CA:1489:G:O2'   | 1:CA:1490:C:H5'   | 2.14                     | 0.48              |
| 1:CA:571:U:H3'    | 1:CA:572:A:H5''   | 1.96                     | 0.48              |
| 1:CA:571:U:H5''   | 1:CA:819:A:N3     | 2.29                     | 0.48              |
| 3:CC:156:ARG:HH11 | 3:CC:193:TYR:HB2  | 1.77                     | 0.48              |
| 4:CD:99:SER:O     | 4:CD:140:VAL:HG23 | 2.14                     | 0.48              |
| 4:CD:177:ASP:O    | 4:CD:177:ASP:OD1  | 2.31                     | 0.48              |
| 5:CE:53:LEU:CD1   | 5:CE:53:LEU:H     | 2.24                     | 0.48              |
| 5:CE:67:VAL:CG2   | 5:CE:68:GLU:N     | 2.75                     | 0.48              |
| 23:CW:70:C:O2'    | 23:CW:71:A:C5'    | 2.62                     | 0.48              |
| 52:D3:31:LEU:C    | 52:D3:33:GLN:H    | 2.17                     | 0.48              |
| 45:DW:35:ILE:HG23 | 54:D5:28:PRO:CD   | 2.43                     | 0.48              |
| 55:D6:34:LEU:N    | 55:D6:51:GLU:OE1  | 2.47                     | 0.48              |
| 27:DA:997:G:C2    | 27:DA:1159:U:N3   | 2.82                     | 0.48              |
| 27:DA:1354:A:H2'  | 27:DA:1355:G:O4'  | 2.14                     | 0.48              |
| 27:DA:1385:G:C4   | 27:DA:1386:C:C5   | 3.02                     | 0.48              |
| 27:DA:1479:G:H2'  | 27:DA:1480:G:H8   | 1.78                     | 0.48              |
| 27:DA:1332:G:N2   | 27:DA:1609:A:HO2' | 2.12                     | 0.48              |
| 27:DA:199:A:C5    | 27:DA:2434:A:N6   | 2.81                     | 0.48              |
| 27:DA:2003:G:C2'  | 27:DA:2004:G:O5'  | 2.62                     | 0.48              |
| 27:DA:2011:U:H2'  | 27:DA:2012:G:O4'  | 2.14                     | 0.48              |
| 27:DA:2203:U:H1'  | 30:DD:151:LYS:HE3 | 1.96                     | 0.48              |
| 27:DA:921:G:H4'   | 27:DA:2269:A:C6   | 2.49                     | 0.48              |
| 27:DA:2527:C:C4   | 27:DA:2528:U:C5   | 3.01                     | 0.48              |
| 27:DA:2544:G:C4   | 27:DA:2545:G:C8   | 3.02                     | 0.48              |
| 27:DA:2566:A:O2'  | 27:DA:2567:G:P    | 2.72                     | 0.48              |
| 27:DA:2653:U:H3'  | 27:DA:2654:A:H8   | 1.79                     | 0.48              |
| 27:DA:2817:G:C2   | 27:DA:2818:G:H1'  | 2.49                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2849:U:O2'   | 27:DA:2866:U:C6    | 2.67                     | 0.48              |
| 27:DA:324:A:N6     | 27:DA:338:G:O2'    | 2.37                     | 0.48              |
| 27:DA:71:A:C4'     | 27:DA:72:U:OP2     | 2.62                     | 0.48              |
| 27:DA:736:C:C2'    | 27:DA:737:C:H5'    | 2.44                     | 0.48              |
| 27:DA:849:A:OP2    | 27:DA:850:C:C5     | 2.67                     | 0.48              |
| 27:DA:997:G:OP1    | 43:DU:93:LYS:HD3   | 2.13                     | 0.48              |
| 28:DB:46:A:C5      | 28:DB:47:C:C4      | 3.01                     | 0.48              |
| 28:DB:21:G:H1      | 28:DB:62:C:H42     | 1.61                     | 0.48              |
| 31:DE:59:VAL:CG2   | 31:DE:60:ASN:H     | 2.06                     | 0.48              |
| 33:DG:125:PHE:CD1  | 33:DG:125:PHE:N    | 2.82                     | 0.48              |
| 36:DN:38:HIS:HA    | 43:DU:67:ALA:HB1   | 1.96                     | 0.48              |
| 39:DQ:34:LEU:HB2   | 39:DQ:118:LEU:HD22 | 1.96                     | 0.48              |
| 42:DT:13:ARG:C     | 42:DT:15:VAL:H     | 2.17                     | 0.48              |
| 42:DT:96:ARG:CG    | 42:DT:96:ARG:NH1   | 2.70                     | 0.48              |
| 36:DN:2:LYS:HE2    | 43:DU:95:LEU:HD21  | 1.95                     | 0.48              |
| 45:DW:105:VAL:HG12 | 45:DW:107:LEU:HD12 | 1.95                     | 0.48              |
| 45:DW:50:VAL:HG13  | 45:DW:51:LEU:N     | 2.23                     | 0.48              |
| 48:DZ:120:HIS:C    | 48:DZ:122:ASP:H    | 2.17                     | 0.48              |
| 1:AA:1009:G:H2'    | 1:AA:1009:G:N3     | 2.28                     | 0.48              |
| 1:AA:145:G:H5'     | 1:AA:146:G:OP2     | 2.13                     | 0.48              |
| 3:AC:133:ALA:O     | 3:AC:137:ALA:N     | 2.45                     | 0.48              |
| 1:AA:559:A:OP1     | 5:AE:126:ARG:NH2   | 2.46                     | 0.48              |
| 6:AF:75:LEU:C      | 6:AF:77:ARG:N      | 2.67                     | 0.48              |
| 8:AH:118:VAL:C     | 8:AH:119:LEU:HD23  | 2.33                     | 0.48              |
| 8:AH:85:ARG:HH11   | 8:AH:85:ARG:HG3    | 1.78                     | 0.48              |
| 9:AI:23:ASN:HB2    | 9:AI:60:ASP:CG     | 2.33                     | 0.48              |
| 10:AJ:54:PHE:CG    | 10:AJ:55:LYS:HE3   | 2.49                     | 0.48              |
| 10:AJ:5:ARG:HG2    | 10:AJ:6:ILE:N      | 2.28                     | 0.48              |
| 14:AN:13:THR:O     | 14:AN:14:PRO:C     | 2.51                     | 0.48              |
| 16:AP:72:ARG:O     | 16:AP:75:ARG:HB3   | 2.14                     | 0.48              |
| 17:AQ:22:LEU:HA    | 17:AQ:22:LEU:HD12  | 1.65                     | 0.48              |
| 18:AR:63:GLN:OE1   | 18:AR:66:LEU:HD23  | 2.14                     | 0.48              |
| 20:AT:58:LYS:O     | 20:AT:61:SER:HB3   | 2.13                     | 0.48              |
| 24:AX:17:C:H2'     | 24:AX:17(B):U:C6   | 2.48                     | 0.48              |
| 49:B0:66:VAL:N     | 49:B0:82:ARG:O     | 2.46                     | 0.48              |
| 53:B4:62:CYS:SG    | 53:B4:63:SER:N     | 2.87                     | 0.48              |
| 57:B8:10:ALA:O     | 57:B8:11:LYS:C     | 2.52                     | 0.48              |
| 27:BA:1441:G:H2'   | 27:BA:1442:G:C8    | 2.40                     | 0.48              |
| 27:BA:1961:C:H2'   | 27:BA:1962:C:H5'   | 1.96                     | 0.48              |
| 27:BA:2109:U:N3    | 27:BA:2110:G:O6    | 2.46                     | 0.48              |
| 27:BA:2266:A:H4'   | 27:BA:2267:A:H5'   | 1.96                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:2736:G:O2'   | 27:BA:2737:G:H5'  | 2.14                     | 0.48              |
| 27:BA:415:A:H2'    | 27:BA:416:C:C6    | 2.49                     | 0.48              |
| 27:BA:552:G:C6     | 27:BA:553:G:C5    | 3.02                     | 0.48              |
| 27:BA:560:C:C2'    | 27:BA:561:G:O5'   | 2.62                     | 0.48              |
| 27:BA:840:C:H2'    | 27:BA:841:A:C8    | 2.49                     | 0.48              |
| 28:BB:24:G:H4'     | 28:BB:25:A:C5'    | 2.44                     | 0.48              |
| 29:BC:184:LYS:C    | 29:BC:186:ALA:N   | 2.67                     | 0.48              |
| 30:BD:222:ARG:HH21 | 30:BD:225:ALA:HB2 | 1.78                     | 0.48              |
| 30:BD:44:ASN:CB    | 30:BD:48:ARG:O    | 2.59                     | 0.48              |
| 31:BE:78:LEU:C     | 31:BE:79:ARG:HD2  | 2.34                     | 0.48              |
| 33:BG:142:PRO:HG2  | 33:BG:143:GLU:H   | 1.78                     | 0.48              |
| 33:BG:81:LYS:O     | 33:BG:82:LEU:O    | 2.32                     | 0.48              |
| 34:BH:24:VAL:HG23  | 34:BH:24:VAL:O    | 2.14                     | 0.48              |
| 37:BO:10:VAL:HG23  | 37:BO:10:VAL:O    | 2.14                     | 0.48              |
| 37:BO:10:VAL:HG22  | 37:BO:17:ARG:O    | 2.13                     | 0.48              |
| 39:BQ:43:THR:OG1   | 39:BQ:46:GLN:NE2  | 2.47                     | 0.48              |
| 39:BQ:89:ASN:HB2   | 39:BQ:91:GLU:OE2  | 2.14                     | 0.48              |
| 40:BR:18:LEU:HD13  | 40:BR:18:LEU:C    | 2.33                     | 0.48              |
| 40:BR:33:ARG:HD2   | 40:BR:33:ARG:N    | 2.29                     | 0.48              |
| 42:BT:31:SER:O     | 42:BT:82:LEU:HA   | 2.13                     | 0.48              |
| 27:BA:2012:G:C3'   | 45:BW:96:ILE:HD11 | 2.43                     | 0.48              |
| 1:CA:1290:G:H3'    | 1:CA:1291:G:H8    | 1.78                     | 0.48              |
| 1:CA:369:C:N3      | 1:CA:393:A:C2     | 2.81                     | 0.48              |
| 1:CA:540:G:C4      | 1:CA:541:G:C8     | 3.01                     | 0.48              |
| 1:CA:600:C:H2'     | 1:CA:601:C:C6     | 2.49                     | 0.48              |
| 1:CA:834:C:C2'     | 1:CA:835:U:O5'    | 2.62                     | 0.48              |
| 2:CB:9:GLU:O       | 2:CB:12:GLU:OE1   | 2.32                     | 0.48              |
| 3:CC:44:GLU:HG3    | 3:CC:52:LEU:HD11  | 1.96                     | 0.48              |
| 3:CC:83:ARG:NH1    | 3:CC:83:ARG:HG2   | 2.28                     | 0.48              |
| 4:CD:114:ARG:O     | 4:CD:117:ALA:HB3  | 2.14                     | 0.48              |
| 4:CD:11:LEU:O      | 4:CD:12:CYS:C     | 2.52                     | 0.48              |
| 6:CF:19:LEU:HD11   | 6:CF:59:TYR:CE2   | 2.48                     | 0.48              |
| 7:CG:83:ALA:O      | 7:CG:85:TYR:N     | 2.47                     | 0.48              |
| 8:CH:84:ARG:O      | 8:CH:135:CYS:HB2  | 2.13                     | 0.48              |
| 12:CL:120:LYS:O    | 12:CL:121:LYS:C   | 2.51                     | 0.48              |
| 15:CO:21:ASP:OD2   | 15:CO:24:SER:HB2  | 2.12                     | 0.48              |
| 15:CO:2:PRO:CG     | 15:CO:3:ILE:H     | 2.25                     | 0.48              |
| 17:CQ:12:SER:HA    | 17:CQ:14:LYS:HZ1  | 1.77                     | 0.48              |
| 18:CR:75:ILE:C     | 18:CR:77:GLY:H    | 2.14                     | 0.48              |
| 24:CX:39:C:O2'     | 25:CY:33:G:N2     | 2.46                     | 0.48              |
| 56:D7:12:ARG:HD3   | 56:D7:46:VAL:CG2  | 2.43                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 58:D9:22:ARG:HD3   | 58:D9:35:ARG:HD2    | 1.95                     | 0.48              |
| 27:DA:1022:G:O2'   | 27:DA:1023:U:OP2    | 2.32                     | 0.48              |
| 27:DA:1230:C:O2'   | 27:DA:1231:G:H5'    | 2.13                     | 0.48              |
| 27:DA:1237:A:H2    | 27:DA:1238:G:C2     | 2.31                     | 0.48              |
| 27:DA:1322:A:C5    | 27:DA:1323:U:C5     | 3.02                     | 0.48              |
| 27:DA:131:G:C2     | 27:DA:132:G:C5      | 3.02                     | 0.48              |
| 27:DA:1444:G:N1    | 27:DA:1548:C:N4     | 2.62                     | 0.48              |
| 27:DA:1567:A:H4'   | 30:DD:58:HIS:NE2    | 2.29                     | 0.48              |
| 27:DA:157:U:O4'    | 27:DA:157:U:P       | 2.72                     | 0.48              |
| 27:DA:2189:U:H5'   | 27:DA:2190:G:OP2    | 2.14                     | 0.48              |
| 27:DA:2206:G:N2    | 27:DA:2207:G:H4'    | 2.28                     | 0.48              |
| 27:DA:397:G:H5''   | 50:D1:45:ASN:HB3    | 1.94                     | 0.48              |
| 27:DA:783:A:C2     | 27:DA:785:G:H1'     | 2.48                     | 0.48              |
| 27:DA:807:U:OP2    | 38:DP:39:LYS:HD2    | 2.13                     | 0.48              |
| 27:DA:856:C:H5''   | 27:DA:856:C:C6      | 2.49                     | 0.48              |
| 27:DA:887:A:H1'    | 27:DA:889:C:C4      | 2.49                     | 0.48              |
| 29:DC:129:ARG:C    | 29:DC:131:LEU:H     | 2.17                     | 0.48              |
| 30:DD:123:ALA:HB3  | 30:DD:131:LEU:HG    | 1.95                     | 0.48              |
| 30:DD:67:PHE:CG    | 30:DD:153:ALA:HB3   | 2.49                     | 0.48              |
| 32:DF:36:VAL:CG1   | 32:DF:183:VAL:HG21  | 2.36                     | 0.48              |
| 33:DG:53:LEU:N     | 33:DG:53:LEU:HD22   | 2.28                     | 0.48              |
| 35:DI:29:TYR:CE2   | 35:DI:35:LEU:HD12   | 2.49                     | 0.48              |
| 38:DP:9:ASN:N      | 38:DP:10:PRO:CD     | 2.72                     | 0.48              |
| 27:DA:671:C:H5     | 38:DP:36:LYS:HE2    | 1.79                     | 0.48              |
| 43:DU:15:LYS:HG2   | 43:DU:15:LYS:O      | 2.13                     | 0.48              |
| 43:DU:34:LYS:HA    | 43:DU:34:LYS:CE     | 2.44                     | 0.48              |
| 47:DY:53:PRO:HB3   | 47:DY:56:PRO:O      | 2.13                     | 0.48              |
| 1:AA:1030(A):G:H2' | 1:AA:1030(B):C:H5'' | 1.95                     | 0.48              |
| 1:AA:1229:A:N6     | 13:AM:105:THR:HG22  | 2.28                     | 0.48              |
| 1:AA:405:U:O2      | 1:AA:498:U:C6       | 2.67                     | 0.48              |
| 1:AA:713:G:O2'     | 1:AA:714:G:H5'      | 2.14                     | 0.48              |
| 1:AA:839:U:O2      | 1:AA:839:U:C2'      | 2.62                     | 0.48              |
| 1:AA:917:G:C6      | 1:AA:918:A:C6       | 3.02                     | 0.48              |
| 2:AB:200:ILE:O     | 2:AB:201:ILE:HD13   | 2.14                     | 0.48              |
| 2:AB:97:TRP:HH2    | 2:AB:176:GLU:CD     | 2.17                     | 0.48              |
| 3:AC:134:ILE:O     | 3:AC:136:GLN:N      | 2.47                     | 0.48              |
| 1:AA:1205:U:H4'    | 3:AC:195:VAL:CG2    | 2.44                     | 0.48              |
| 3:AC:58:GLU:N      | 3:AC:65:ALA:HB3     | 2.29                     | 0.48              |
| 10:AJ:32:ALA:HB3   | 10:AJ:75:ILE:CG1    | 2.44                     | 0.48              |
| 13:AM:11:ARG:O     | 13:AM:13:LYS:N      | 2.47                     | 0.48              |
| 17:AQ:89:LEU:O     | 17:AQ:93:GLN:HG3    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1457:G:P     | 20:AT:39:LYS:HZ2  | 2.36                     | 0.48              |
| 20:AT:77:ALA:C    | 20:AT:79:ARG:H    | 2.16                     | 0.48              |
| 23:AW:40:C:O2'    | 23:AW:41:G:H5'    | 2.14                     | 0.48              |
| 49:B0:31:VAL:HB   | 49:B0:35:ASN:HD22 | 1.78                     | 0.48              |
| 50:B1:7:ILE:HD13  | 50:B1:62:VAL:HG23 | 1.96                     | 0.48              |
| 53:B4:51:TYR:N    | 53:B4:51:TYR:CD1  | 2.82                     | 0.48              |
| 27:BA:1556:C:C2'  | 27:BA:1557:C:H6   | 2.27                     | 0.48              |
| 27:BA:192:C:C2'   | 27:BA:193:U:H5'   | 2.42                     | 0.48              |
| 27:BA:2628:C:H4'  | 27:BA:2781:A:C6   | 2.49                     | 0.48              |
| 27:BA:2716:U:H2'  | 27:BA:2717:G:C8   | 2.49                     | 0.48              |
| 27:BA:424:G:O2'   | 27:BA:425:G:H5'   | 2.13                     | 0.48              |
| 27:BA:42:G:C2     | 27:BA:43:A:H1'    | 2.49                     | 0.48              |
| 27:BA:947:G:H2'   | 27:BA:948:G:H8    | 1.77                     | 0.48              |
| 31:BE:11:MET:HB3  | 31:BE:24:THR:HA   | 1.95                     | 0.48              |
| 31:BE:60:ASN:OD1  | 31:BE:62:PRO:HD2  | 2.14                     | 0.48              |
| 34:BH:147:ASN:O   | 34:BH:150:ALA:CB  | 2.61                     | 0.48              |
| 34:BH:156:ALA:N   | 34:BH:158:HIS:H   | 2.10                     | 0.48              |
| 37:BO:87:ILE:HG21 | 37:BO:91:LEU:HA   | 1.95                     | 0.48              |
| 39:BQ:76:LYS:HG3  | 39:BQ:77:LYS:O    | 2.14                     | 0.48              |
| 43:BU:40:PHE:O    | 43:BU:41:ALA:C    | 2.52                     | 0.48              |
| 46:BX:31:HIS:HD2  | 46:BX:32:PRO:CD   | 2.27                     | 0.48              |
| 47:BY:51:VAL:O    | 47:BY:52:SER:HB3  | 2.14                     | 0.48              |
| 48:BZ:150:HIS:HA  | 48:BZ:169:THR:HA  | 1.96                     | 0.48              |
| 1:CA:1036:G:H3'   | 1:CA:1037:C:C6    | 2.49                     | 0.48              |
| 1:CA:10:A:H2'     | 1:CA:11:G:H8      | 1.79                     | 0.48              |
| 1:CA:1253:G:H2'   | 1:CA:1254:C:C6    | 2.49                     | 0.48              |
| 1:CA:1286:A:H2    | 21:CU:22:ARG:NH2  | 2.10                     | 0.48              |
| 1:CA:132:C:H5'    | 1:CA:262:A:H1'    | 1.95                     | 0.48              |
| 1:CA:335:C:H2'    | 1:CA:336:C:H6     | 1.75                     | 0.48              |
| 1:CA:349:A:C2'    | 1:CA:350:G:H5'    | 2.44                     | 0.48              |
| 1:CA:590:C:C4     | 1:CA:650:G:N1     | 2.82                     | 0.48              |
| 1:CA:794:A:O2'    | 1:CA:795:C:H5'    | 2.14                     | 0.48              |
| 1:CA:815:A:H5'    | 1:CA:816:A:C5'    | 2.44                     | 0.48              |
| 1:CA:935:A:O2'    | 1:CA:936:C:P      | 2.72                     | 0.48              |
| 2:CB:77:ALA:O     | 2:CB:81:VAL:HG23  | 2.14                     | 0.48              |
| 3:CC:122:GLU:O    | 3:CC:126:ARG:HG3  | 2.14                     | 0.48              |
| 3:CC:14:ILE:CG1   | 3:CC:15:THR:H     | 2.18                     | 0.48              |
| 4:CD:110:PHE:HD1  | 4:CD:110:PHE:H    | 1.60                     | 0.48              |
| 4:CD:98:GLU:OE1   | 4:CD:194:LEU:HD11 | 2.14                     | 0.48              |
| 4:CD:5:ILE:H      | 4:CD:115:ARG:HH12 | 1.62                     | 0.48              |
| 4:CD:78:LEU:O     | 4:CD:79:PHE:C     | 2.52                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CF:23:LYS:HG2    | 6:CF:61:LEU:HD21   | 1.96                     | 0.48              |
| 1:CA:1346:A:C5     | 7:CG:10:ARG:NH2    | 2.82                     | 0.48              |
| 8:CH:86:ILE:HB     | 8:CH:133:LEU:CD2   | 2.43                     | 0.48              |
| 11:CK:16:SER:O     | 11:CK:35:PRO:HG3   | 2.14                     | 0.48              |
| 14:CN:24:CYS:HB3   | 14:CN:27:CYS:O     | 2.12                     | 0.48              |
| 16:CP:53:VAL:HG12  | 16:CP:79:VAL:HG22  | 1.95                     | 0.48              |
| 19:CS:9:VAL:C      | 19:CS:11:VAL:N     | 2.68                     | 0.48              |
| 20:CT:81:LYS:O     | 20:CT:85:MET:HG2   | 2.14                     | 0.48              |
| 57:D8:23:VAL:CG1   | 57:D8:46:ARG:HB3   | 2.43                     | 0.48              |
| 27:DA:1152:C:H1'   | 43:DU:77:SER:CB    | 2.44                     | 0.48              |
| 27:DA:140:G:N2     | 27:DA:142:A:C2     | 2.75                     | 0.48              |
| 27:DA:1700:A:O2'   | 27:DA:1701:A:O4'   | 2.32                     | 0.48              |
| 27:DA:1830:C:N4    | 27:DA:1975:G:H1    | 2.11                     | 0.48              |
| 27:DA:2156:G:C5    | 27:DA:2157:G:N2    | 2.82                     | 0.48              |
| 27:DA:2175:C:H1'   | 29:DC:215:THR:HA   | 1.95                     | 0.48              |
| 27:DA:2177:C:O2'   | 27:DA:2178:C:H5'   | 2.14                     | 0.48              |
| 27:DA:2271:G:C5    | 27:DA:2272:U:C5    | 3.02                     | 0.48              |
| 27:DA:2299:G:C2    | 27:DA:2318:G:H8    | 2.32                     | 0.48              |
| 27:DA:2428:G:H21   | 38:DP:60:MET:CE    | 2.27                     | 0.48              |
| 27:DA:2556:C:H2'   | 27:DA:2557:G:O4'   | 2.14                     | 0.48              |
| 27:DA:2508:G:C2    | 27:DA:2582:G:C6    | 3.02                     | 0.48              |
| 27:DA:2787:C:O2    | 31:DE:61:ARG:NH1   | 2.46                     | 0.48              |
| 27:DA:796:C:H2'    | 27:DA:797:C:H6     | 1.71                     | 0.48              |
| 27:DA:859:G:H22    | 27:DA:916:G:H3'    | 1.79                     | 0.48              |
| 27:DA:920:G:H8     | 27:DA:920:G:O5'    | 1.97                     | 0.48              |
| 27:DA:953:A:C2     | 27:DA:954:G:C8     | 3.02                     | 0.48              |
| 31:DE:176:ILE:HG22 | 31:DE:176:ILE:O    | 2.13                     | 0.48              |
| 32:DF:89:VAL:CG1   | 32:DF:90:PHE:H     | 2.20                     | 0.48              |
| 37:DO:35:VAL:HG13  | 37:DO:62:VAL:HG12  | 1.96                     | 0.48              |
| 38:DP:144:GLU:O    | 38:DP:145:PRO:C    | 2.53                     | 0.48              |
| 40:DR:26:LYS:HE2   | 40:DR:71:GLN:N     | 2.27                     | 0.48              |
| 41:DS:87:PHE:CD1   | 41:DS:106:ARG:NH2  | 2.81                     | 0.48              |
| 41:DS:10:ARG:O     | 41:DS:11:LYS:O     | 2.31                     | 0.48              |
| 42:DT:55:ASN:C     | 42:DT:55:ASN:HD22  | 2.17                     | 0.48              |
| 44:DV:75:PHE:CE2   | 44:DV:82:ARG:NE    | 2.78                     | 0.48              |
| 45:DW:54:ALA:O     | 45:DW:57:ASN:HB2   | 2.14                     | 0.48              |
| 47:DY:95:LYS:CG    | 47:DY:100:ALA:HA   | 2.44                     | 0.48              |
| 48:DZ:150:HIS:CD2  | 48:DZ:169:THR:HG22 | 2.48                     | 0.48              |
| 1:AA:1054:C:N3     | 23:AW:33:C:H1'     | 2.29                     | 0.47              |
| 1:AA:1275:A:H2'    | 1:AA:1276:G:H8     | 1.79                     | 0.47              |
| 1:AA:1281:U:O4     | 10:AJ:7:LYS:NZ     | 2.37                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1431:C:H2'   | 1:AA:1432:G:O4'   | 2.14                     | 0.47              |
| 1:AA:1442:G:H1    | 1:AA:1461:G:H21   | 1.62                     | 0.47              |
| 1:AA:434:U:C2'    | 1:AA:435:C:O4'    | 2.61                     | 0.47              |
| 1:AA:865:A:H5'    | 1:AA:1078:U:C5    | 2.49                     | 0.47              |
| 2:AB:144:ARG:O    | 2:AB:145:LEU:C    | 2.52                     | 0.47              |
| 4:AD:200:GLU:HG2  | 4:AD:201:GLN:N    | 2.28                     | 0.47              |
| 5:AE:109:ILE:O    | 5:AE:113:ALA:N    | 2.47                     | 0.47              |
| 12:AL:25:LYS:CE   | 12:AL:30:ARG:HH22 | 2.27                     | 0.47              |
| 12:AL:86:ARG:CA   | 12:AL:94:ARG:HA   | 2.44                     | 0.47              |
| 13:AM:19:LEU:HD11 | 13:AM:56:LEU:HD11 | 1.96                     | 0.47              |
| 1:AA:974:A:P      | 14:AN:29:ARG:HH22 | 2.37                     | 0.47              |
| 17:AQ:59:ILE:HA   | 17:AQ:72:ARG:O    | 2.14                     | 0.47              |
| 17:AQ:58:GLU:O    | 17:AQ:73:VAL:HA   | 2.14                     | 0.47              |
| 20:AT:73:HIS:O    | 20:AT:74:LYS:O    | 2.31                     | 0.47              |
| 23:AW:4:G:H3'     | 23:AW:5:G:H5''    | 1.96                     | 0.47              |
| 24:AX:25:C:H2'    | 24:AX:26:G:C8     | 2.48                     | 0.47              |
| 51:B2:28:LYS:HB2  | 51:B2:57:ILE:HD12 | 1.96                     | 0.47              |
| 53:B4:62:CYS:SG   | 53:B4:64:LYS:CB   | 3.02                     | 0.47              |
| 55:B6:42:TRP:CE3  | 55:B6:42:TRP:HA   | 2.49                     | 0.47              |
| 56:B7:11:LYS:O    | 56:B7:12:ARG:C    | 2.52                     | 0.47              |
| 56:B7:35:ARG:HG3  | 56:B7:42:LEU:HD21 | 1.96                     | 0.47              |
| 27:BA:1303:G:C2   | 27:BA:1304:C:C6   | 3.02                     | 0.47              |
| 27:BA:1310:G:H2'  | 27:BA:1311:G:H5'  | 1.96                     | 0.47              |
| 27:BA:1315:C:O2   | 27:BA:1392:A:H2   | 1.97                     | 0.47              |
| 27:BA:1797:C:O2   | 27:BA:1823:G:C2   | 2.67                     | 0.47              |
| 27:BA:1963:U:OP1  | 27:BA:1963:U:H3'  | 2.13                     | 0.47              |
| 27:BA:196:A:C5    | 27:BA:805:G:C6    | 3.02                     | 0.47              |
| 27:BA:1984:G:O2'  | 27:BA:1985:G:H5'  | 2.14                     | 0.47              |
| 27:BA:2091:U:O4   | 27:BA:2092:U:C4   | 2.67                     | 0.47              |
| 27:BA:2305:A:C2   | 27:BA:2306:C:H1'  | 2.49                     | 0.47              |
| 27:BA:2354:G:H2'  | 27:BA:2355:C:C6   | 2.48                     | 0.47              |
| 27:BA:242:G:C5'   | 57:B8:62:LEU:HD22 | 2.44                     | 0.47              |
| 27:BA:2884:U:O2   | 54:B5:51:TYR:CE1  | 2.66                     | 0.47              |
| 27:BA:340:A:H2'   | 27:BA:341:G:O4'   | 2.14                     | 0.47              |
| 27:BA:922:U:C2    | 27:BA:923:C:C5    | 3.01                     | 0.47              |
| 28:BB:105:A:C2'   | 28:BB:106:G:C5'   | 2.90                     | 0.47              |
| 29:BC:47:LEU:CB   | 29:BC:207:THR:HA  | 2.44                     | 0.47              |
| 30:BD:227:ASN:HB3 | 30:BD:228:PRO:CD  | 2.44                     | 0.47              |
| 31:BE:63:LEU:O    | 31:BE:64:LYS:C    | 2.52                     | 0.47              |
| 33:BG:2:PRO:C     | 33:BG:4:ASP:N     | 2.60                     | 0.47              |
| 33:BG:60:LEU:C    | 33:BG:62:LEU:H    | 2.17                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BS:85:VAL:O    | 41:BS:86:ALA:HB2  | 2.14                     | 0.47              |
| 42:BT:92:GLY:O    | 42:BT:93:ARG:HB3  | 2.13                     | 0.47              |
| 44:BV:81:TYR:CE2  | 44:BV:83:ARG:HG3  | 2.49                     | 0.47              |
| 45:BW:14:PRO:O    | 45:BW:15:ARG:C    | 2.52                     | 0.47              |
| 46:BX:31:HIS:HD2  | 46:BX:33:LYS:H    | 1.57                     | 0.47              |
| 48:BZ:103:PHE:N   | 48:BZ:103:PHE:CD1 | 2.82                     | 0.47              |
| 48:BZ:150:HIS:CA  | 48:BZ:169:THR:HA  | 2.44                     | 0.47              |
| 1:CA:1028:C:C2'   | 1:CA:1029:C:H5'   | 2.44                     | 0.47              |
| 1:CA:1057:G:H2'   | 1:CA:1058:G:O5'   | 2.14                     | 0.47              |
| 1:CA:1068:G:C8    | 1:CA:1094:G:C8    | 3.02                     | 0.47              |
| 1:CA:1199:U:H5''  | 1:CA:1200:C:OP2   | 2.13                     | 0.47              |
| 1:CA:949:A:C2     | 1:CA:1233:G:N3    | 2.82                     | 0.47              |
| 1:CA:1383:C:O2'   | 1:CA:1384:C:H5'   | 2.13                     | 0.47              |
| 1:CA:197:A:O2'    | 1:CA:198:G:O4'    | 2.31                     | 0.47              |
| 1:CA:338:A:H61    | 1:CA:351:G:H1     | 1.62                     | 0.47              |
| 1:CA:471:G:C2'    | 1:CA:472:A:H8     | 2.26                     | 0.47              |
| 1:CA:520:A:N1     | 1:CA:536:C:O2     | 2.47                     | 0.47              |
| 1:CA:984:C:O2'    | 1:CA:985:C:C6     | 2.65                     | 0.47              |
| 2:CB:100:GLY:O    | 2:CB:104:ASN:N    | 2.46                     | 0.47              |
| 1:CA:1106:G:OP1   | 3:CC:172:ARG:HD3  | 2.14                     | 0.47              |
| 4:CD:101:LEU:HD23 | 4:CD:138:TYR:HB3  | 1.96                     | 0.47              |
| 4:CD:68:TYR:O     | 4:CD:69:GLY:C     | 2.52                     | 0.47              |
| 8:CH:28:ALA:HA    | 8:CH:59:LEU:HG    | 1.96                     | 0.47              |
| 11:CK:15:ALA:HB1  | 11:CK:78:GLN:HB2  | 1.95                     | 0.47              |
| 14:CN:23:ARG:O    | 14:CN:24:CYS:C    | 2.51                     | 0.47              |
| 1:CA:1186:G:H21   | 14:CN:61:TRP:C    | 2.17                     | 0.47              |
| 15:CO:65:ARG:NH1  | 15:CO:65:ARG:HG2  | 2.28                     | 0.47              |
| 17:CQ:20:THR:HA   | 17:CQ:43:LEU:CD2  | 2.44                     | 0.47              |
| 20:CT:63:ILE:HD13 | 20:CT:80:ARG:HB3  | 1.96                     | 0.47              |
| 25:CY:52:G:N2     | 25:CY:60:C:O2     | 2.47                     | 0.47              |
| 51:D2:31:GLU:O    | 51:D2:34:GLU:N    | 2.47                     | 0.47              |
| 27:DA:1025:G:HO2' | 27:DA:1026:U:P    | 2.36                     | 0.47              |
| 27:DA:1037:G:H1   | 27:DA:1118:C:N4   | 2.11                     | 0.47              |
| 27:DA:2308:G:C5   | 27:DA:2310:A:H5'  | 2.49                     | 0.47              |
| 27:DA:2363:C:H2'  | 27:DA:2364:C:H6   | 1.79                     | 0.47              |
| 25:CY:75:A:C2     | 27:DA:2422:A:C6   | 3.02                     | 0.47              |
| 27:DA:2439:A:H5'  | 27:DA:2439:A:C8   | 2.49                     | 0.47              |
| 27:DA:2653:U:H2'  | 27:DA:2654:A:C8   | 2.49                     | 0.47              |
| 27:DA:27:G:HO2'   | 27:DA:28:A:H8     | 1.62                     | 0.47              |
| 27:DA:34:C:O2'    | 27:DA:35:G:C5'    | 2.52                     | 0.47              |
| 27:DA:475:U:H2'   | 27:DA:476:G:C8    | 2.49                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:869:G:H5'   | 39:DQ:6:ARG:NH2    | 2.28                     | 0.47              |
| 30:DD:72:LYS:CE   | 30:DD:101:GLU:OE2  | 2.58                     | 0.47              |
| 30:DD:20:ASP:C    | 30:DD:20:ASP:OD1   | 2.52                     | 0.47              |
| 31:DE:34:VAL:HG23 | 31:DE:48:GLN:HG2   | 1.96                     | 0.47              |
| 31:DE:84:PHE:CD2  | 31:DE:84:PHE:C     | 2.87                     | 0.47              |
| 32:DF:108:LYS:HB3 | 32:DF:112:MET:HE2  | 1.96                     | 0.47              |
| 32:DF:152:GLU:HB3 | 32:DF:191:ARG:HD2  | 1.96                     | 0.47              |
| 33:DG:152:LEU:HG  | 33:DG:153:ARG:N    | 2.29                     | 0.47              |
| 35:DI:43:ASN:O    | 35:DI:44:LEU:C     | 2.52                     | 0.47              |
| 35:DI:54:GLN:O    | 35:DI:58:LEU:HB2   | 2.14                     | 0.47              |
| 35:DI:68:LEU:C    | 35:DI:68:LEU:HD23  | 2.34                     | 0.47              |
| 37:DO:101:PRO:O   | 37:DO:102:VAL:HG12 | 2.14                     | 0.47              |
| 38:DP:58:THR:O    | 38:DP:61:ARG:HG3   | 2.14                     | 0.47              |
| 27:DA:518:G:H4'   | 45:DW:18:ARG:NH2   | 2.29                     | 0.47              |
| 46:DX:63:LYS:HA   | 46:DX:72:LYS:HA    | 1.96                     | 0.47              |
| 48:DZ:2:TYR:O     | 48:DZ:56:ILE:HA    | 2.14                     | 0.47              |
| 1:AA:260:G:H2'    | 1:AA:261:U:C6      | 2.48                     | 0.47              |
| 1:AA:255:G:O6     | 1:AA:266:G:O6      | 2.33                     | 0.47              |
| 1:AA:415:A:H2'    | 1:AA:416:G:H8      | 1.77                     | 0.47              |
| 1:AA:823:G:H2'    | 1:AA:824:C:O4'     | 2.14                     | 0.47              |
| 1:AA:859:A:C2'    | 1:AA:860:A:H5'     | 2.44                     | 0.47              |
| 1:AA:953:G:H5''   | 1:AA:965:A:H61     | 1.78                     | 0.47              |
| 2:AB:55:PHE:C     | 2:AB:57:PHE:N      | 2.67                     | 0.47              |
| 3:AC:188:LEU:HD12 | 3:AC:195:VAL:HG11  | 1.96                     | 0.47              |
| 3:AC:92:ALA:CB    | 3:AC:99:VAL:HG11   | 2.40                     | 0.47              |
| 5:AE:101:ILE:N    | 5:AE:101:ILE:CD1   | 2.67                     | 0.47              |
| 9:AI:28:VAL:HG11  | 9:AI:36:TYR:CE2    | 2.50                     | 0.47              |
| 12:AL:24:LEU:C    | 12:AL:26:GLY:N     | 2.67                     | 0.47              |
| 15:AO:23:GLY:O    | 15:AO:27:VAL:HB    | 2.14                     | 0.47              |
| 18:AR:32:ARG:NH1  | 18:AR:65:ILE:HD13  | 2.29                     | 0.47              |
| 18:AR:46:GLU:HB2  | 18:AR:85:LEU:HD21  | 1.96                     | 0.47              |
| 20:AT:96:GLY:O    | 20:AT:97:ALA:O     | 2.33                     | 0.47              |
| 24:AX:40:C:H2'    | 24:AX:41:C:H6      | 1.77                     | 0.47              |
| 55:B6:27:LYS:CB   | 55:B6:29:ASN:OD1   | 2.61                     | 0.47              |
| 56:B7:8:ASN:CG    | 56:B7:11:LYS:HB3   | 2.35                     | 0.47              |
| 57:B8:4:MET:O     | 57:B8:62:LEU:CD1   | 2.62                     | 0.47              |
| 27:BA:1048:A:O2'  | 27:BA:1049:C:P     | 2.71                     | 0.47              |
| 27:BA:1170:G:N2   | 27:BA:1180:C:C2    | 2.82                     | 0.47              |
| 27:BA:1847:A:C4'  | 27:BA:1848:A:OP2   | 2.62                     | 0.47              |
| 27:BA:1980:G:O2'  | 27:BA:1982:C:OP2   | 2.30                     | 0.47              |
| 27:BA:2302:G:H21  | 33:BG:128:ARG:CG   | 2.26                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2317:C:C3'  | 27:BA:2318:G:H5'   | 2.41                     | 0.47              |
| 27:BA:2366:A:H2'  | 27:BA:2367:G:O4'   | 2.13                     | 0.47              |
| 27:BA:2370:G:H2'  | 27:BA:2371:G:C8    | 2.48                     | 0.47              |
| 27:BA:2427:C:C5'  | 27:BA:2429:G:H5'   | 2.44                     | 0.47              |
| 27:BA:2458:G:H2'  | 27:BA:2490:G:H1    | 1.80                     | 0.47              |
| 27:BA:2729:G:H4'  | 31:BE:185:LYS:O    | 2.13                     | 0.47              |
| 27:BA:381:G:OP1   | 50:B1:16:ASN:ND2   | 2.47                     | 0.47              |
| 27:BA:925:C:C2'   | 27:BA:926:A:O5'    | 2.62                     | 0.47              |
| 28:BB:1:U:C5      | 28:BB:2:C:C4       | 3.01                     | 0.47              |
| 28:BB:51:G:OP2    | 41:BS:61:ASN:O     | 2.32                     | 0.47              |
| 28:BB:87:G:H3'    | 28:BB:88:C:C5'     | 2.44                     | 0.47              |
| 30:BD:112:GLN:HB2 | 30:BD:115:GLN:NE2  | 2.24                     | 0.47              |
| 31:BE:49:LEU:CD1  | 31:BE:49:LEU:N     | 2.77                     | 0.47              |
| 32:BF:22:ALA:CA   | 32:BF:26:ALA:HB2   | 2.44                     | 0.47              |
| 27:BA:588:U:H1'   | 32:BF:90:PHE:CG    | 2.50                     | 0.47              |
| 33:BG:110:ALA:HB2 | 33:BG:141:PHE:HA   | 1.96                     | 0.47              |
| 33:BG:83:ARG:HH11 | 33:BG:84:LYS:HD2   | 1.79                     | 0.47              |
| 33:BG:9:ARG:O     | 33:BG:11:TYR:N     | 2.47                     | 0.47              |
| 34:BH:13:LYS:HD3  | 34:BH:14:GLY:H     | 1.76                     | 0.47              |
| 34:BH:155:SER:OG  | 34:BH:156:ALA:N    | 2.47                     | 0.47              |
| 34:BH:85:LYS:NZ   | 34:BH:133:VAL:CG2  | 2.73                     | 0.47              |
| 37:BO:38:VAL:O    | 37:BO:39:ILE:CG2   | 2.62                     | 0.47              |
| 38:BP:9:ASN:H     | 38:BP:10:PRO:CD    | 2.27                     | 0.47              |
| 27:BA:2710:C:OP1  | 40:BR:15:SER:HB2   | 2.14                     | 0.47              |
| 43:BU:18:LEU:O    | 43:BU:19:LYS:C     | 2.52                     | 0.47              |
| 43:BU:21:ALA:HB1  | 43:BU:24:TYR:CE1   | 2.49                     | 0.47              |
| 48:BZ:129:PRO:HA  | 48:BZ:132:ILE:HD11 | 1.96                     | 0.47              |
| 1:CA:1020:U:H2'   | 1:CA:1021:G:H8     | 1.80                     | 0.47              |
| 1:CA:1367:C:OP1   | 9:CI:115:GLY:N     | 2.44                     | 0.47              |
| 1:CA:1390:U:H2'   | 1:CA:1391:U:C6     | 2.44                     | 0.47              |
| 1:CA:321:A:O5'    | 1:CA:321:A:H8      | 1.96                     | 0.47              |
| 1:CA:472:A:O2'    | 1:CA:473:G:H5'     | 2.14                     | 0.47              |
| 1:CA:545:C:C4     | 1:CA:546:G:N7      | 2.82                     | 0.47              |
| 1:CA:834:C:H42    | 1:CA:852:G:H1      | 1.62                     | 0.47              |
| 1:CA:867:G:H21    | 1:CA:873:A:H2      | 1.62                     | 0.47              |
| 1:CA:862:C:H1'    | 1:CA:874:G:H4'     | 1.95                     | 0.47              |
| 1:CA:76:C:N4      | 1:CA:93:G:H1       | 2.12                     | 0.47              |
| 1:CA:942:G:C6     | 1:CA:1342:C:N3     | 2.81                     | 0.47              |
| 2:CB:10:LEU:O     | 2:CB:14:GLY:N      | 2.47                     | 0.47              |
| 4:CD:101:LEU:HA   | 4:CD:140:VAL:CG2   | 2.44                     | 0.47              |
| 4:CD:112:VAL:HG12 | 4:CD:161:ASN:ND2   | 2.29                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:CD:137:SER:O     | 4:CD:138:TYR:C    | 2.52                     | 0.47              |
| 10:CJ:94:VAL:CG1   | 10:CJ:95:GLU:N    | 2.77                     | 0.47              |
| 17:CQ:84:LEU:HA    | 17:CQ:87:LYS:HG2  | 1.96                     | 0.47              |
| 1:CA:191:G:O2'     | 20:CT:102:GLY:O   | 2.30                     | 0.47              |
| 50:D1:58:ILE:HD12  | 50:D1:60:PHE:HE2  | 1.79                     | 0.47              |
| 50:D1:8:SER:HB3    | 50:D1:66:HIS:CD2  | 2.49                     | 0.47              |
| 46:DX:5:TYR:CE2    | 51:D2:30:ARG:HB2  | 2.49                     | 0.47              |
| 57:D8:40:GLU:C     | 57:D8:42:ARG:N    | 2.67                     | 0.47              |
| 58:D9:29:ASN:H     | 58:D9:29:ASN:HD22 | 1.61                     | 0.47              |
| 27:DA:106:C:O4'    | 47:DY:2:ARG:HG3   | 2.15                     | 0.47              |
| 27:DA:1127:A:C2'   | 27:DA:1128:A:H5'' | 2.43                     | 0.47              |
| 27:DA:1416:G:O2'   | 27:DA:1417:C:C6   | 2.54                     | 0.47              |
| 27:DA:768:G:H5'    | 27:DA:1622:G:H4'  | 1.97                     | 0.47              |
| 27:DA:1824:G:N3    | 30:DD:254:THR:OG1 | 2.47                     | 0.47              |
| 27:DA:1924:C:N4    | 27:DA:1925:C:N4   | 2.62                     | 0.47              |
| 27:DA:2249:U:H1'   | 27:DA:2275:C:N4   | 2.28                     | 0.47              |
| 27:DA:2423:U:O3'   | 27:DA:2425:A:H2'  | 2.14                     | 0.47              |
| 27:DA:2473:U:C2'   | 27:DA:2473:U:O2   | 2.54                     | 0.47              |
| 27:DA:295:G:H2'    | 27:DA:295:G:N3    | 2.29                     | 0.47              |
| 27:DA:529:A:C5'    | 27:DA:530:G:OP1   | 2.61                     | 0.47              |
| 27:DA:553:G:C2'    | 27:DA:554:U:H5'   | 2.44                     | 0.47              |
| 27:DA:723:G:C2     | 27:DA:724:U:C2    | 3.03                     | 0.47              |
| 27:DA:8:A:H2'      | 27:DA:9:U:C5      | 2.46                     | 0.47              |
| 27:DA:970:C:O2     | 27:DA:984:A:O2'   | 2.29                     | 0.47              |
| 28:DB:104:U:O2'    | 28:DB:105:A:H5'   | 2.14                     | 0.47              |
| 29:DC:168:THR:HA   | 29:DC:173:ALA:HB1 | 1.96                     | 0.47              |
| 30:DD:206:LEU:HD22 | 30:DD:211:ARG:HG2 | 1.96                     | 0.47              |
| 35:DI:25:TYR:HE2   | 35:DI:29:TYR:CD2  | 2.32                     | 0.47              |
| 36:DN:111:PRO:HA   | 36:DN:114:ARG:NH2 | 2.28                     | 0.47              |
| 38:DP:32:THR:O     | 38:DP:33:ARG:CB   | 2.62                     | 0.47              |
| 38:DP:48:PRO:O     | 38:DP:50:ARG:N    | 2.46                     | 0.47              |
| 39:DQ:79:LEU:CD2   | 39:DQ:80:GLU:N    | 2.77                     | 0.47              |
| 41:DS:106:ARG:O    | 41:DS:107:GLU:CB  | 2.62                     | 0.47              |
| 41:DS:69:VAL:O     | 41:DS:70:GLY:C    | 2.52                     | 0.47              |
| 41:DS:85:VAL:HB    | 41:DS:86:ALA:H    | 1.49                     | 0.47              |
| 42:DT:129:ARG:CZ   | 42:DT:131:ALA:O   | 2.62                     | 0.47              |
| 42:DT:28:VAL:HG11  | 42:DT:46:GLU:CD   | 2.34                     | 0.47              |
| 43:DU:111:GLU:O    | 43:DU:112:ARG:C   | 2.51                     | 0.47              |
| 43:DU:79:PHE:HD2   | 43:DU:83:LEU:HD13 | 1.80                     | 0.47              |
| 45:DW:51:LEU:C     | 45:DW:51:LEU:HD13 | 2.34                     | 0.47              |
| 45:DW:59:VAL:HG12  | 45:DW:60:ASN:HD22 | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:DW:85:VAL:HG13 | 45:DW:86:LEU:N    | 2.28                     | 0.47              |
| 46:DX:36:LYS:O    | 46:DX:39:ILE:HB   | 2.14                     | 0.47              |
| 47:DY:14:LEU:HD12 | 47:DY:15:VAL:N    | 2.28                     | 0.47              |
| 48:DZ:51:SER:OG   | 48:DZ:52:ILE:N    | 2.47                     | 0.47              |
| 1:AA:1225:A:OP2   | 1:AA:1226:C:C5    | 2.63                     | 0.47              |
| 1:AA:1340:A:C2'   | 1:AA:1341:U:H5'   | 2.44                     | 0.47              |
| 2:AB:121:LEU:O    | 2:AB:121:LEU:HD23 | 2.14                     | 0.47              |
| 8:AH:104:ARG:HD3  | 8:AH:138:TRP:CG   | 2.48                     | 0.47              |
| 8:AH:9:MET:HE3    | 8:AH:35:ILE:HG21  | 1.95                     | 0.47              |
| 9:AI:45:ALA:O     | 9:AI:48:GLU:HB2   | 2.14                     | 0.47              |
| 9:AI:95:LYS:CG    | 9:AI:96:LEU:N     | 2.77                     | 0.47              |
| 10:AJ:88:LEU:HG   | 10:AJ:88:LEU:O    | 2.14                     | 0.47              |
| 12:AL:21:VAL:O    | 12:AL:21:VAL:HG12 | 2.14                     | 0.47              |
| 12:AL:55:VAL:O    | 12:AL:62:GLU:HA   | 2.14                     | 0.47              |
| 13:AM:76:ALA:O    | 13:AM:79:LYS:N    | 2.46                     | 0.47              |
| 14:AN:23:ARG:O    | 14:AN:24:CYS:C    | 2.52                     | 0.47              |
| 15:AO:35:ARG:NH1  | 15:AO:59:MET:SD   | 2.87                     | 0.47              |
| 17:AQ:58:GLU:OE1  | 17:AQ:75:ARG:NE   | 2.48                     | 0.47              |
| 19:AS:79:THR:O    | 19:AS:80:TYR:HB2  | 2.15                     | 0.47              |
| 25:AY:19:U:H2'    | 25:AY:20:A:H4'    | 1.94                     | 0.47              |
| 25:AY:69:C:H5'    | 25:AY:69:C:H6     | 1.79                     | 0.47              |
| 50:B1:53:VAL:HG21 | 50:B1:74:VAL:HG22 | 1.95                     | 0.47              |
| 51:B2:28:LYS:O    | 51:B2:53:LEU:HD11 | 2.14                     | 0.47              |
| 38:BP:61:ARG:HD3  | 57:B8:13:ARG:HD2  | 1.95                     | 0.47              |
| 27:BA:1505:C:H3'  | 27:BA:1506:C:C6   | 2.49                     | 0.47              |
| 27:BA:1909:C:H2'  | 27:BA:1909:C:O2   | 2.13                     | 0.47              |
| 27:BA:1925:C:H2'  | 27:BA:1926:U:O5'  | 2.14                     | 0.47              |
| 27:BA:1935:G:O2'  | 27:BA:1936:A:H5'  | 2.13                     | 0.47              |
| 27:BA:1996:C:C4'  | 27:BA:1997:G:O5'  | 2.62                     | 0.47              |
| 27:BA:2092:U:O2   | 27:BA:2092:U:O4'  | 2.31                     | 0.47              |
| 27:BA:2266:A:H5'' | 27:BA:2267:A:H5'' | 1.96                     | 0.47              |
| 27:BA:2286:A:H5'' | 27:BA:2287:A:O5'  | 2.14                     | 0.47              |
| 27:BA:2285:C:O2'  | 27:BA:2288:A:H2'  | 2.14                     | 0.47              |
| 27:BA:2352:A:H2'  | 27:BA:2353:G:H5'  | 1.94                     | 0.47              |
| 27:BA:2670:A:H2'  | 27:BA:2671:A:H5'  | 1.96                     | 0.47              |
| 27:BA:355:G:H2'   | 27:BA:356:G:C1'   | 2.44                     | 0.47              |
| 27:BA:181:A:C4    | 27:BA:435:C:C6    | 3.02                     | 0.47              |
| 27:BA:652:C:C6    | 27:BA:652:C:H5''  | 2.49                     | 0.47              |
| 27:BA:69:C:H4'    | 27:BA:75:G:C5     | 2.48                     | 0.47              |
| 27:BA:750:A:H2'   | 27:BA:751:A:H5''  | 1.96                     | 0.47              |
| 27:BA:985:C:C2    | 27:BA:986:C:C5    | 3.02                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:764:A:C6    | 30:BD:209:ALA:CB  | 2.97                     | 0.47              |
| 31:BE:187:ALA:O   | 31:BE:188:VAL:C   | 2.50                     | 0.47              |
| 33:BG:130:ASN:HB3 | 33:BG:160:VAL:HA  | 1.96                     | 0.47              |
| 33:BG:73:ALA:O    | 33:BG:85:GLY:HA2  | 2.14                     | 0.47              |
| 34:BH:88:LEU:HD13 | 34:BH:130:ARG:HG3 | 1.94                     | 0.47              |
| 38:BP:81:GLN:OE1  | 38:BP:106:LEU:HA  | 2.14                     | 0.47              |
| 44:BV:41:GLY:CA   | 44:BV:45:THR:OG1  | 2.46                     | 0.47              |
| 45:BW:111:HIS:CD2 | 45:BW:112:GLY:N   | 2.83                     | 0.47              |
| 46:BX:28:PHE:N    | 46:BX:28:PHE:CD1  | 2.82                     | 0.47              |
| 46:BX:26:TYR:HD2  | 46:BX:92:LEU:HD12 | 1.79                     | 0.47              |
| 47:BY:28:LYS:N    | 47:BY:28:LYS:HE3  | 2.29                     | 0.47              |
| 47:BY:81:LYS:HZ2  | 47:BY:97:ARG:CG   | 2.26                     | 0.47              |
| 1:CA:1050:G:H2'   | 1:CA:1051:C:H6    | 1.78                     | 0.47              |
| 1:CA:495:A:C2     | 1:CA:496:A:C2     | 3.03                     | 0.47              |
| 1:CA:499:A:H4'    | 1:CA:500:G:OP1    | 2.14                     | 0.47              |
| 1:CA:538:G:C4'    | 12:CL:111:LYS:HD3 | 2.45                     | 0.47              |
| 1:CA:557:G:H3'    | 1:CA:558:G:C8     | 2.49                     | 0.47              |
| 1:CA:831:U:OP1    | 2:CB:22:LYS:HD2   | 2.14                     | 0.47              |
| 2:CB:120:ALA:C    | 2:CB:122:PHE:N    | 2.66                     | 0.47              |
| 2:CB:239:VAL:O    | 2:CB:241:GLU:N    | 2.47                     | 0.47              |
| 3:CC:173:VAL:HG12 | 3:CC:175:LEU:CD1  | 2.44                     | 0.47              |
| 6:CF:49:ALA:HB3   | 18:CR:79:LEU:O    | 2.14                     | 0.47              |
| 7:CG:145:ALA:O    | 7:CG:146:GLU:CB   | 2.59                     | 0.47              |
| 9:CI:55:ALA:HB2   | 9:CI:59:PHE:HE1   | 1.79                     | 0.47              |
| 9:CI:7:THR:O      | 9:CI:79:LEU:HD12  | 2.12                     | 0.47              |
| 9:CI:82:ALA:CB    | 9:CI:96:LEU:HD11  | 2.33                     | 0.47              |
| 10:CJ:56:HIS:O    | 10:CJ:58:ASP:N    | 2.47                     | 0.47              |
| 10:CJ:80:LYS:HE3  | 10:CJ:80:LYS:O    | 2.15                     | 0.47              |
| 12:CL:114:ARG:HB2 | 12:CL:114:ARG:CZ  | 2.45                     | 0.47              |
| 13:CM:80:ARG:C    | 13:CM:82:MET:H    | 2.17                     | 0.47              |
| 14:CN:59:ALA:O    | 14:CN:60:SER:HB2  | 2.14                     | 0.47              |
| 16:CP:17:TYR:N    | 16:CP:17:TYR:CD1  | 2.81                     | 0.47              |
| 18:CR:66:LEU:HD12 | 18:CR:70:ILE:HG12 | 1.95                     | 0.47              |
| 50:D1:24:ALA:HB3  | 50:D1:27:GLU:CD   | 2.34                     | 0.47              |
| 27:DA:2396:G:H1'  | 50:D1:30:VAL:HG13 | 1.96                     | 0.47              |
| 57:D8:52:LYS:O    | 57:D8:55:ALA:HB3  | 2.13                     | 0.47              |
| 27:DA:1170:G:H22  | 27:DA:1179:C:N4   | 2.11                     | 0.47              |
| 27:DA:1236:G:OP2  | 27:DA:1236:G:H8   | 1.97                     | 0.47              |
| 27:DA:1754:C:H5'' | 42:DT:113:LYS:HZ2 | 1.79                     | 0.47              |
| 27:DA:1831:G:C6   | 27:DA:1832:C:C4   | 3.03                     | 0.47              |
| 27:DA:1925:C:H2'  | 27:DA:1926:U:H5'  | 1.95                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:2018:G:H2'   | 27:DA:2019:A:O4'  | 2.14                     | 0.47              |
| 27:DA:2303:G:H2'   | 27:DA:2304:G:C8   | 2.48                     | 0.47              |
| 27:DA:2373:G:C2'   | 27:DA:2374:C:H5'  | 2.44                     | 0.47              |
| 27:DA:2509:G:C4    | 27:DA:2510:C:C5   | 3.02                     | 0.47              |
| 27:DA:2515:C:H2'   | 27:DA:2516:G:C8   | 2.44                     | 0.47              |
| 27:DA:2520:C:H2'   | 27:DA:2521:C:O4'  | 2.15                     | 0.47              |
| 27:DA:266:G:C2'    | 27:DA:267:C:O5'   | 2.63                     | 0.47              |
| 27:DA:317:G:H2'    | 27:DA:318:C:O4'   | 2.13                     | 0.47              |
| 27:DA:35:G:O2'     | 27:DA:454:A:O4'   | 2.31                     | 0.47              |
| 27:DA:639:U:C4     | 27:DA:640:C:N4    | 2.82                     | 0.47              |
| 27:DA:873:G:H4'    | 39:DQ:63:LYS:CE   | 2.44                     | 0.47              |
| 28:DB:110:G:O2'    | 28:DB:111:G:H5'   | 2.13                     | 0.47              |
| 30:DD:70:TRP:CZ2   | 30:DD:150:LYS:HA  | 2.49                     | 0.47              |
| 33:DG:77:ILE:N     | 33:DG:83:ARG:HB3  | 2.25                     | 0.47              |
| 34:DH:105:LEU:CD2  | 34:DH:105:LEU:N   | 2.77                     | 0.47              |
| 36:DN:112:LEU:HA   | 36:DN:115:ARG:HB3 | 1.95                     | 0.47              |
| 37:DO:100:GLY:O    | 37:DO:101:PRO:O   | 2.31                     | 0.47              |
| 40:DR:2:ARG:HH21   | 40:DR:5:LYS:HZ1   | 1.60                     | 0.47              |
| 43:DU:100:VAL:HG12 | 43:DU:101:ARG:N   | 2.28                     | 0.47              |
| 36:DN:2:LYS:HZ1    | 44:DV:13:ARG:H    | 1.62                     | 0.47              |
| 44:DV:34:GLU:O     | 44:DV:36:PRO:CD   | 2.62                     | 0.47              |
| 1:AA:328:C:O2      | 1:AA:328:C:C2'    | 2.62                     | 0.47              |
| 1:AA:642:A:H2'     | 1:AA:643:C:H6     | 1.79                     | 0.47              |
| 1:AA:643:C:C2'     | 1:AA:644:G:H5'    | 2.43                     | 0.47              |
| 3:AC:24:ALA:HB1    | 3:AC:29:TYR:HA    | 1.97                     | 0.47              |
| 3:AC:42:LEU:HA     | 3:AC:45:LYS:CD    | 2.45                     | 0.47              |
| 4:AD:20:TYR:CD2    | 4:AD:27:TYR:CE2   | 3.02                     | 0.47              |
| 6:AF:1:MET:HE2     | 6:AF:68:PRO:HA    | 1.96                     | 0.47              |
| 9:AI:77:ILE:HG22   | 9:AI:81:ILE:HG12  | 1.97                     | 0.47              |
| 13:AM:20:THR:C     | 13:AM:22:ILE:H    | 2.15                     | 0.47              |
| 13:AM:76:ALA:HB2   | 13:AM:79:LYS:NZ   | 2.28                     | 0.47              |
| 15:AO:62:GLN:HA    | 15:AO:65:ARG:NH1  | 2.23                     | 0.47              |
| 19:AS:28:LYS:HB3   | 19:AS:29:ARG:H    | 1.42                     | 0.47              |
| 23:AW:59:U:H5'     | 23:AW:60:C:OP2    | 2.14                     | 0.47              |
| 27:BA:1400:G:C6    | 27:BA:1401:G:C6   | 3.03                     | 0.47              |
| 27:BA:1714:G:H2'   | 27:BA:1717:G:O4'  | 2.13                     | 0.47              |
| 27:BA:2050:C:H2'   | 27:BA:2051:A:C8   | 2.50                     | 0.47              |
| 27:BA:2115:G:O5'   | 27:BA:2115:G:H8   | 1.97                     | 0.47              |
| 27:BA:180:G:N2     | 27:BA:215:G:O6    | 2.47                     | 0.47              |
| 27:BA:215:G:H4'    | 27:BA:216:A:O5'   | 2.14                     | 0.47              |
| 27:BA:2416:C:OP1   | 38:BP:64:LYS:O    | 2.32                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:2772:C:N3    | 27:BA:2773:C:C4   | 2.83                     | 0.47              |
| 27:BA:664:C:H1'    | 27:BA:940:G:OP1   | 2.14                     | 0.47              |
| 27:BA:666:G:O2'    | 27:BA:667:U:H5'   | 2.15                     | 0.47              |
| 27:BA:795:C:C2     | 27:BA:796:C:C5    | 3.02                     | 0.47              |
| 27:BA:83:G:O2'     | 27:BA:84:A:OP2    | 2.32                     | 0.47              |
| 27:BA:943:U:H2'    | 27:BA:944:G:O4'   | 2.14                     | 0.47              |
| 27:BA:971:C:O2'    | 27:BA:972:G:H5'   | 2.15                     | 0.47              |
| 28:BB:12:C:H6      | 28:BB:12:C:OP2    | 1.97                     | 0.47              |
| 30:BD:134:ARG:HG2  | 30:BD:135:PHE:CD1 | 2.50                     | 0.47              |
| 31:BE:171:GLU:HB3  | 31:BE:185:LYS:HG2 | 1.96                     | 0.47              |
| 32:BF:192:LEU:HD23 | 32:BF:192:LEU:C   | 2.33                     | 0.47              |
| 34:BH:157:TYR:O    | 34:BH:158:HIS:HD2 | 1.97                     | 0.47              |
| 35:BI:82:ARG:O     | 35:BI:88:ILE:CG2  | 2.62                     | 0.47              |
| 36:BN:86:PRO:O     | 36:BN:89:LYS:HB2  | 2.14                     | 0.47              |
| 39:BQ:135:ASP:HB2  | 39:BQ:136:ALA:H   | 1.52                     | 0.47              |
| 42:BT:125:ARG:O    | 42:BT:128:GLU:CG  | 2.54                     | 0.47              |
| 44:BV:47:VAL:O     | 44:BV:49:THR:O    | 2.32                     | 0.47              |
| 45:BW:88:ARG:HB2   | 45:BW:92:ARG:CB   | 2.30                     | 0.47              |
| 48:BZ:30:ARG:HG2   | 48:BZ:30:ARG:O    | 2.13                     | 0.47              |
| 1:CA:1117:G:H21    | 1:CA:1180:A:H1'   | 1.79                     | 0.47              |
| 1:CA:1336:C:H4'    | 1:CA:1337:G:N3    | 2.30                     | 0.47              |
| 1:CA:1488:G:O2'    | 1:CA:1489:G:H5'   | 2.13                     | 0.47              |
| 1:CA:223:U:H2'     | 1:CA:224:C:C6     | 2.49                     | 0.47              |
| 1:CA:584:G:O2'     | 1:CA:585:G:H5'    | 2.15                     | 0.47              |
| 2:CB:142:LEU:HD11  | 2:CB:146:GLN:HB2  | 1.97                     | 0.47              |
| 5:CE:103:GLY:C     | 5:CE:105:VAL:N    | 2.68                     | 0.47              |
| 10:CJ:78:ASN:ND2   | 10:CJ:80:LYS:CB   | 2.77                     | 0.47              |
| 11:CK:48:ILE:O     | 11:CK:50:TYR:N    | 2.48                     | 0.47              |
| 16:CP:4:ILE:HG12   | 16:CP:21:VAL:CG2  | 2.40                     | 0.47              |
| 17:CQ:76:LEU:O     | 17:CQ:76:LEU:HG   | 2.14                     | 0.47              |
| 23:CW:30:A:H2'     | 23:CW:31:U:H5'    | 1.95                     | 0.47              |
| 25:CY:21:A:H8      | 25:CY:21:A:OP2    | 1.98                     | 0.47              |
| 49:D0:51:VAL:HG23  | 49:D0:81:VAL:HG23 | 1.95                     | 0.47              |
| 56:D7:28:ARG:O     | 56:D7:31:LEU:N    | 2.47                     | 0.47              |
| 27:DA:1051:G:H21   | 27:DA:1052:C:H6   | 1.60                     | 0.47              |
| 27:DA:1053:C:O2    | 27:DA:1053:C:C2'  | 2.62                     | 0.47              |
| 27:DA:1159:U:H5''  | 27:DA:1159:U:H6   | 1.79                     | 0.47              |
| 27:DA:181:A:H1'    | 27:DA:435:C:H5''  | 1.96                     | 0.47              |
| 27:DA:2184:G:H2'   | 27:DA:2185:C:C6   | 2.49                     | 0.47              |
| 27:DA:2400:G:O2'   | 55:D6:19:ARG:HG3  | 2.14                     | 0.47              |
| 27:DA:2542:A:C8    | 27:DA:2544:G:O6   | 2.67                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:307:G:N1     | 27:DA:310:A:OP2   | 2.45                     | 0.47              |
| 27:DA:527:C:O4'    | 27:DA:527:C:O2    | 2.31                     | 0.47              |
| 27:DA:531:C:OP1    | 27:DA:561:G:N2    | 2.47                     | 0.47              |
| 27:DA:779:U:O4     | 27:DA:780:G:C6    | 2.67                     | 0.47              |
| 27:DA:955:C:H5''   | 39:DQ:87:LYS:HE2  | 1.96                     | 0.47              |
| 28:DB:47:C:C2'     | 28:DB:48:A:H5'    | 2.44                     | 0.47              |
| 29:DC:49:ILE:HG22  | 29:DC:50:ASP:OD1  | 2.14                     | 0.47              |
| 30:DD:16:MET:HA    | 30:DD:205:VAL:O   | 2.15                     | 0.47              |
| 30:DD:221:VAL:HG23 | 30:DD:226:MET:CE  | 2.44                     | 0.47              |
| 30:DD:61:LEU:CB    | 30:DD:63:ARG:NH1  | 2.70                     | 0.47              |
| 30:DD:70:TRP:O     | 30:DD:73:VAL:CG2  | 2.63                     | 0.47              |
| 30:DD:94:LEU:HB2   | 30:DD:104:TYR:CE2 | 2.49                     | 0.47              |
| 31:DE:197:ILE:HG13 | 31:DE:198:VAL:N   | 2.26                     | 0.47              |
| 32:DF:110:LEU:HD13 | 32:DF:110:LEU:C   | 2.34                     | 0.47              |
| 33:DG:39:ILE:HG22  | 33:DG:92:VAL:O    | 2.14                     | 0.47              |
| 35:DI:1:MET:O      | 35:DI:20:ASP:HA   | 2.14                     | 0.47              |
| 27:DA:1138:G:N2    | 36:DN:106:MET:SD  | 2.80                     | 0.47              |
| 38:DP:30:THR:CG2   | 38:DP:31:ALA:H    | 2.27                     | 0.47              |
| 27:DA:997:G:OP1    | 43:DU:93:LYS:HB2  | 2.14                     | 0.47              |
| 36:DN:2:LYS:HZ1    | 44:DV:13:ARG:N    | 2.12                     | 0.47              |
| 45:DW:59:VAL:HG12  | 45:DW:60:ASN:N    | 2.29                     | 0.47              |
| 45:DW:73:ALA:O     | 45:DW:106:ILE:CG1 | 2.53                     | 0.47              |
| 48:DZ:167:GLU:O    | 48:DZ:168:GLU:C   | 2.52                     | 0.47              |
| 1:AA:198:G:O2'     | 1:AA:199:G:O4'    | 2.29                     | 0.47              |
| 1:AA:60:A:OP2      | 1:AA:387:U:H4'    | 2.15                     | 0.47              |
| 2:AB:122:PHE:HD1   | 2:AB:139:LYS:NZ   | 2.12                     | 0.47              |
| 2:AB:236:TYR:CD1   | 2:AB:236:TYR:N    | 2.82                     | 0.47              |
| 4:AD:68:TYR:HA     | 4:AD:114:ARG:HD3  | 1.96                     | 0.47              |
| 5:AE:37:ARG:O      | 5:AE:38:GLN:HG2   | 2.15                     | 0.47              |
| 7:AG:95:ARG:NH1    | 7:AG:99:LEU:HD21  | 2.29                     | 0.47              |
| 8:AH:124:ALA:HB1   | 8:AH:129:VAL:HG23 | 1.97                     | 0.47              |
| 8:AH:84:ARG:NH1    | 8:AH:84:ARG:CB    | 2.78                     | 0.47              |
| 9:AI:118:LYS:O     | 9:AI:120:ARG:N    | 2.40                     | 0.47              |
| 11:AK:76:GLY:O     | 11:AK:77:MET:O    | 2.32                     | 0.47              |
| 13:AM:3:ARG:HB2    | 53:B4:60:GLU:HG2  | 1.95                     | 0.47              |
| 16:AP:71:ARG:O     | 16:AP:75:ARG:N    | 2.45                     | 0.47              |
| 50:B1:70:VAL:C     | 50:B1:72:GLU:N    | 2.68                     | 0.47              |
| 50:B1:53:VAL:HG22  | 50:B1:74:VAL:HG13 | 1.95                     | 0.47              |
| 51:B2:9:GLN:NE2    | 51:B2:56:GLN:HG2  | 2.29                     | 0.47              |
| 52:B3:30:ARG:HD3   | 52:B3:33:GLN:HE21 | 1.79                     | 0.47              |
| 27:BA:1222:C:C2    | 27:BA:1223:G:C8   | 3.02                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1314:C:H2'   | 27:BA:1315:C:H6    | 1.79                     | 0.47              |
| 27:BA:1434:A:H2'   | 27:BA:1435:G:C8    | 2.49                     | 0.47              |
| 27:BA:1515:G:O2'   | 27:BA:1516:C:H5'   | 2.14                     | 0.47              |
| 27:BA:1835:G:N3    | 27:BA:1835:G:C2'   | 2.76                     | 0.47              |
| 27:BA:2437:U:C2    | 27:BA:2438:U:C5    | 3.02                     | 0.47              |
| 23:AW:75:A:H4'     | 27:BA:2506:U:O2'   | 2.15                     | 0.47              |
| 27:BA:2787:C:O2    | 27:BA:2787:C:C2'   | 2.62                     | 0.47              |
| 27:BA:286:C:C2     | 27:BA:356:G:C2     | 3.03                     | 0.47              |
| 27:BA:717:G:C6     | 27:BA:718:A:C4     | 3.02                     | 0.47              |
| 27:BA:7:G:H2'      | 27:BA:8:A:H8       | 1.73                     | 0.47              |
| 27:BA:80:G:C2'     | 27:BA:81:G:H5'     | 2.44                     | 0.47              |
| 27:BA:951:C:H6     | 27:BA:951:C:O5'    | 1.97                     | 0.47              |
| 30:BD:142:VAL:HG21 | 30:BD:191:ALA:HB1  | 1.96                     | 0.47              |
| 30:BD:214:TRP:C    | 30:BD:216:GLY:H    | 2.16                     | 0.47              |
| 27:BA:1822:G:O3'   | 30:BD:54:ARG:NH2   | 2.47                     | 0.47              |
| 31:BE:203:LYS:CD   | 31:BE:203:LYS:O    | 2.58                     | 0.47              |
| 31:BE:65:GLY:O     | 31:BE:66:HIS:C     | 2.53                     | 0.47              |
| 31:BE:32:PRO:HB3   | 31:BE:69:LYS:HG2   | 1.96                     | 0.47              |
| 32:BF:182:ASN:ND2  | 32:BF:185:ASP:OD2  | 2.44                     | 0.47              |
| 32:BF:1:MET:CG     | 32:BF:26:ALA:HA    | 2.44                     | 0.47              |
| 27:BA:449:A:OP1    | 32:BF:84:VAL:O     | 2.32                     | 0.47              |
| 34:BH:115:VAL:HG21 | 34:BH:148:ILE:HD11 | 1.97                     | 0.47              |
| 35:BI:89:TYR:C     | 35:BI:121:LYS:HZ2  | 2.17                     | 0.47              |
| 35:BI:77:LEU:HD13  | 35:BI:79:ILE:HD11  | 1.97                     | 0.47              |
| 27:BA:636:G:OP2    | 38:BP:131:SER:HA   | 2.14                     | 0.47              |
| 38:BP:132:LYS:H    | 38:BP:132:LYS:HG2  | 1.48                     | 0.47              |
| 40:BR:87:TYR:HE1   | 40:BR:117:VAL:O    | 1.97                     | 0.47              |
| 41:BS:30:ARG:HH22  | 41:BS:62:LYS:CD    | 2.19                     | 0.47              |
| 1:CA:100:C:H2'     | 1:CA:100:C:O2      | 2.14                     | 0.47              |
| 1:CA:1204:A:OP2    | 14:CN:3:ARG:NH1    | 2.47                     | 0.47              |
| 1:CA:1394:A:H2'    | 1:CA:1501:C:O2'    | 2.14                     | 0.47              |
| 1:CA:372:C:H2'     | 1:CA:387:U:O4      | 2.14                     | 0.47              |
| 1:CA:516:U:O4      | 1:CA:533:A:OP2     | 2.32                     | 0.47              |
| 3:CC:119:ARG:NH1   | 3:CC:119:ARG:HG3   | 2.29                     | 0.47              |
| 3:CC:11:ARG:NH1    | 3:CC:11:ARG:HG2    | 2.22                     | 0.47              |
| 3:CC:76:VAL:HG23   | 3:CC:77:ILE:HG13   | 1.97                     | 0.47              |
| 5:CE:148:VAL:O     | 5:CE:152:ARG:HG3   | 2.14                     | 0.47              |
| 5:CE:50:GLU:CB     | 5:CE:53:LEU:HD13   | 2.33                     | 0.47              |
| 6:CF:44:GLY:O      | 6:CF:45:LEU:C      | 2.53                     | 0.47              |
| 7:CG:44:TYR:C      | 7:CG:46:ALA:N      | 2.67                     | 0.47              |
| 7:CG:92:SER:OG     | 7:CG:93:PRO:HD2    | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CH:65:TYR:CD1   | 8:CH:65:TYR:N     | 2.82                     | 0.47              |
| 9:CI:82:ALA:C     | 9:CI:84:ALA:N     | 2.67                     | 0.47              |
| 9:CI:91:ASP:C     | 9:CI:93:ARG:H     | 2.18                     | 0.47              |
| 12:CL:35:THR:CG2  | 12:CL:56:ARG:HH12 | 2.27                     | 0.47              |
| 13:CM:23:TYR:CE1  | 13:CM:70:LEU:CD2  | 2.97                     | 0.47              |
| 1:CA:1188:A:H4'   | 14:CN:58:LYS:NZ   | 2.30                     | 0.47              |
| 15:CO:18:PHE:O    | 15:CO:20:GLY:N    | 2.48                     | 0.47              |
| 15:CO:82:ILE:O    | 15:CO:86:GLY:N    | 2.47                     | 0.47              |
| 17:CQ:60:ILE:C    | 17:CQ:71:PHE:CD1  | 2.87                     | 0.47              |
| 25:CY:18:G:H1'    | 25:CY:56:G:H22    | 1.79                     | 0.47              |
| 27:DA:380:U:H5'   | 50:D1:18:ILE:HD12 | 1.96                     | 0.47              |
| 55:D6:33:LYS:O    | 55:D6:34:LEU:HB2  | 2.13                     | 0.47              |
| 55:D6:40:CYS:HB2  | 55:D6:46:HIS:CG   | 2.49                     | 0.47              |
| 27:DA:592:G:N3    | 57:D8:4:MET:HE2   | 2.30                     | 0.47              |
| 27:DA:1140:C:H1'  | 27:DA:1143:A:N3   | 2.29                     | 0.47              |
| 27:DA:998:C:N4    | 27:DA:1158:C:H42  | 2.13                     | 0.47              |
| 27:DA:1213:A:C4   | 27:DA:1214:A:C8   | 3.03                     | 0.47              |
| 27:DA:146:G:C2    | 27:DA:147:U:C2    | 3.02                     | 0.47              |
| 27:DA:1683:C:N4   | 27:DA:1705:G:H1   | 2.13                     | 0.47              |
| 27:DA:49:A:N6     | 27:DA:177:G:C4    | 2.82                     | 0.47              |
| 27:DA:2118:U:OP1  | 27:DA:2148:G:H4'  | 2.14                     | 0.47              |
| 27:DA:2141:G:C6   | 27:DA:2151:G:C2   | 3.02                     | 0.47              |
| 27:DA:237:C:O2'   | 27:DA:238:C:H5'   | 2.15                     | 0.47              |
| 27:DA:2751:G:N3   | 27:DA:2751:G:C2'  | 2.78                     | 0.47              |
| 27:DA:2848:G:C4'  | 27:DA:2849:U:OP1  | 2.61                     | 0.47              |
| 27:DA:301:G:H1    | 27:DA:316:C:H42   | 1.63                     | 0.47              |
| 27:DA:319:C:H2'   | 27:DA:320:A:C8    | 2.46                     | 0.47              |
| 27:DA:559:G:O2'   | 27:DA:560:C:H5'   | 2.14                     | 0.47              |
| 27:DA:596:G:C6    | 27:DA:597:U:C4    | 3.02                     | 0.47              |
| 27:DA:829:A:H5'   | 27:DA:831:G:N7    | 2.29                     | 0.47              |
| 31:DE:24:THR:HG22 | 31:DE:24:THR:O    | 2.15                     | 0.47              |
| 33:DG:181:ARG:O   | 33:DG:182:LYS:OXT | 2.32                     | 0.47              |
| 33:DG:28:VAL:O    | 33:DG:31:VAL:CG1  | 2.60                     | 0.47              |
| 28:DB:41:U:C5     | 33:DG:69:ALA:HB1  | 2.50                     | 0.47              |
| 39:DQ:58:PHE:HD1  | 39:DQ:58:PHE:O    | 1.96                     | 0.47              |
| 43:DU:79:PHE:CD2  | 43:DU:83:LEU:HD13 | 2.50                     | 0.47              |
| 43:DU:95:LEU:HD13 | 44:DV:4:ILE:CG2   | 2.45                     | 0.47              |
| 44:DV:38:LEU:HD12 | 44:DV:56:SER:C    | 2.35                     | 0.47              |
| 46:DX:78:LYS:O    | 46:DX:78:LYS:HG2  | 2.15                     | 0.47              |
| 1:AA:1152:A:H3'   | 10:AJ:13:HIS:NE2  | 2.30                     | 0.47              |
| 1:AA:246:A:C4'    | 1:AA:247:G:OP1    | 2.62                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:458:C:H2'     | 1:AA:460:G:H8      | 1.80                     | 0.47              |
| 1:AA:663:A:C2'     | 1:AA:664:G:H5'     | 2.44                     | 0.47              |
| 1:AA:835:U:O2'     | 1:AA:836:G:H5'     | 2.14                     | 0.47              |
| 1:AA:864:A:N1      | 1:AA:917:G:O2'     | 2.37                     | 0.47              |
| 1:AA:928:G:H2'     | 1:AA:929:G:C8      | 2.50                     | 0.47              |
| 3:AC:105:GLU:HG2   | 3:AC:106:VAL:H     | 1.80                     | 0.47              |
| 3:AC:61:ALA:O      | 3:AC:62:ASP:HB2    | 2.13                     | 0.47              |
| 4:AD:19:LEU:O      | 4:AD:26:CYS:SG     | 2.72                     | 0.47              |
| 5:AE:130:ASN:C     | 5:AE:132:ALA:N     | 2.65                     | 0.47              |
| 7:AG:23:VAL:O      | 7:AG:24:THR:C      | 2.53                     | 0.47              |
| 8:AH:67:PRO:O      | 8:AH:76:PRO:HB3    | 2.13                     | 0.47              |
| 9:AI:114:TYR:N     | 9:AI:114:TYR:HD2   | 2.13                     | 0.47              |
| 9:AI:14:VAL:O      | 9:AI:65:VAL:HG23   | 2.14                     | 0.47              |
| 10:AJ:83:GLU:HB3   | 10:AJ:84:GLN:NE2   | 2.29                     | 0.47              |
| 10:AJ:95:GLU:OE2   | 10:AJ:95:GLU:HA    | 2.14                     | 0.47              |
| 14:AN:14:PRO:O     | 14:AN:15:LYS:O     | 2.32                     | 0.47              |
| 18:AR:53:ARG:HH21  | 18:AR:60:ALA:N     | 2.07                     | 0.47              |
| 19:AS:27:GLU:O     | 19:AS:28:LYS:O     | 2.33                     | 0.47              |
| 24:AX:12:G:H4'     | 27:BA:1908:C:O2    | 2.14                     | 0.47              |
| 27:BA:1050:A:C4    | 27:BA:1051:G:N7    | 2.83                     | 0.47              |
| 27:BA:1141:U:P     | 36:BN:25:ARG:HH12  | 2.38                     | 0.47              |
| 27:BA:1213:A:C8    | 27:BA:1213:A:C5'   | 2.92                     | 0.47              |
| 27:BA:1380:G:N2    | 27:BA:1570:A:C2    | 2.81                     | 0.47              |
| 27:BA:1632:A:C5    | 27:BA:1633:G:C6    | 3.02                     | 0.47              |
| 27:BA:1945:G:H8    | 27:BA:1945:G:O5'   | 1.98                     | 0.47              |
| 27:BA:1949:G:H2'   | 27:BA:1950:G:C8    | 2.50                     | 0.47              |
| 27:BA:2261:C:C2    | 27:BA:2280:G:C2    | 3.03                     | 0.47              |
| 27:BA:271(J):C:H5' | 27:BA:271(K):U:OP2 | 2.15                     | 0.47              |
| 27:BA:2832:U:O4    | 27:BA:2884:U:C5'   | 2.63                     | 0.47              |
| 27:BA:352:G:C2'    | 27:BA:352:G:N3     | 2.77                     | 0.47              |
| 27:BA:282:A:C4     | 27:BA:359:A:C2     | 3.02                     | 0.47              |
| 27:BA:466:A:C2'    | 27:BA:467:G:H5'    | 2.45                     | 0.47              |
| 27:BA:572:A:H8     | 27:BA:572:A:H5'    | 1.74                     | 0.47              |
| 27:BA:6:A:N3       | 27:BA:6:A:H2'      | 2.29                     | 0.47              |
| 27:BA:859:G:N2     | 27:BA:917:A:OP2    | 2.48                     | 0.47              |
| 30:BD:147:LEU:O    | 30:BD:185:VAL:HG13 | 2.14                     | 0.47              |
| 31:BE:179:GLU:O    | 31:BE:180:ASN:HB2  | 2.13                     | 0.47              |
| 32:BF:35:GLU:O     | 32:BF:38:ARG:HB3   | 2.14                     | 0.47              |
| 33:BG:51:ARG:CA    | 33:BG:51:ARG:NE    | 2.72                     | 0.47              |
| 33:BG:57:ALA:O     | 33:BG:60:LEU:HB3   | 2.14                     | 0.47              |
| 34:BH:68:THR:C     | 34:BH:70:THR:H     | 2.18                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BH:85:LYS:HE2  | 34:BH:145:ALA:N   | 2.29                     | 0.47              |
| 35:BI:12:LEU:CD2  | 35:BI:12:LEU:N    | 2.78                     | 0.47              |
| 35:BI:5:LEU:O     | 35:BI:6:LEU:HD23  | 2.14                     | 0.47              |
| 36:BN:123:TYR:CD1 | 36:BN:123:TYR:N   | 2.82                     | 0.47              |
| 42:BT:34:VAL:HG22 | 42:BT:39:ARG:HG2  | 1.96                     | 0.47              |
| 44:BV:5:VAL:HG11  | 44:BV:57:VAL:CG1  | 2.31                     | 0.47              |
| 45:BW:13:SER:O    | 45:BW:14:PRO:C    | 2.52                     | 0.47              |
| 47:BY:16:ALA:HA   | 47:BY:21:LYS:CD   | 2.45                     | 0.47              |
| 47:BY:81:LYS:HA   | 47:BY:82:PRO:HD3  | 1.78                     | 0.47              |
| 1:CA:55:A:OP2     | 1:CA:352:C:N4     | 2.45                     | 0.47              |
| 1:CA:690:G:H2'    | 1:CA:691:G:C8     | 2.50                     | 0.47              |
| 1:CA:853:G:C4     | 1:CA:854:G:C8     | 3.03                     | 0.47              |
| 1:CA:855:G:C2'    | 1:CA:856:C:H5'    | 2.44                     | 0.47              |
| 1:CA:9:G:O2'      | 1:CA:10:A:O5'     | 2.33                     | 0.47              |
| 4:CD:38:TYR:HB2   | 4:CD:39:PRO:HD2   | 1.97                     | 0.47              |
| 5:CE:90:VAL:O     | 5:CE:91:LEU:HD12  | 2.14                     | 0.47              |
| 7:CG:104:LEU:H    | 7:CG:104:LEU:HD22 | 1.79                     | 0.47              |
| 10:CJ:22:LYS:C    | 10:CJ:24:VAL:H    | 2.18                     | 0.47              |
| 10:CJ:50:ILE:HG21 | 10:CJ:57:LYS:HA   | 1.97                     | 0.47              |
| 11:CK:60:ALA:O    | 11:CK:61:ALA:C    | 2.52                     | 0.47              |
| 13:CM:105:THR:O   | 13:CM:106:ASN:CB  | 2.61                     | 0.47              |
| 1:CA:1310:G:C5'   | 13:CM:77:ASN:HD21 | 2.28                     | 0.47              |
| 14:CN:46:GLU:O    | 14:CN:49:HIS:HB2  | 2.14                     | 0.47              |
| 17:CQ:9:VAL:HG12  | 17:CQ:55:ASP:O    | 2.14                     | 0.47              |
| 17:CQ:7:THR:HG23  | 17:CQ:58:GLU:HG2  | 1.96                     | 0.47              |
| 20:CT:30:LYS:HZ1  | 20:CT:80:ARG:NH2  | 2.12                     | 0.47              |
| 23:CW:18:G:H5'    | 23:CW:59:U:O4     | 2.14                     | 0.47              |
| 55:D6:42:TRP:O    | 55:D6:44:ARG:N    | 2.46                     | 0.47              |
| 27:DA:1279:G:H2'  | 27:DA:1280:G:H8   | 1.78                     | 0.47              |
| 27:DA:1300:U:O2   | 27:DA:1300:U:O4'  | 2.32                     | 0.47              |
| 27:DA:148:C:H2'   | 27:DA:149:A:H5'   | 1.95                     | 0.47              |
| 27:DA:1560:G:H5'  | 27:DA:1560:G:C8   | 2.49                     | 0.47              |
| 27:DA:1792:G:H2'  | 27:DA:1793:C:H6   | 1.79                     | 0.47              |
| 27:DA:1849:G:N3   | 27:DA:1849:G:H2'  | 2.29                     | 0.47              |
| 27:DA:1930:G:N2   | 27:DA:1968:G:H2'  | 2.30                     | 0.47              |
| 27:DA:2016:U:H1'  | 54:D5:6:VAL:CG1   | 2.45                     | 0.47              |
| 27:DA:2077:A:C4   | 27:DA:2435:A:C5   | 3.03                     | 0.47              |
| 27:DA:2334:G:H21  | 41:DS:18:ILE:HD11 | 1.80                     | 0.47              |
| 27:DA:2338:G:O2'  | 27:DA:2339:G:H5'  | 2.15                     | 0.47              |
| 27:DA:2499:C:N4   | 27:DA:2500:U:H3   | 2.13                     | 0.47              |
| 27:DA:2499:C:C4   | 27:DA:2500:U:N3   | 2.82                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:768:G:C6     | 27:DA:769:G:C5     | 3.03                     | 0.47              |
| 27:DA:854:G:O2'    | 27:DA:855:G:H5'    | 2.15                     | 0.47              |
| 27:DA:919:G:C2     | 27:DA:920:G:C4     | 3.02                     | 0.47              |
| 27:DA:969:U:P      | 52:D3:17:LYS:HZ3   | 2.38                     | 0.47              |
| 27:DA:971:C:C2'    | 27:DA:972:G:H5'    | 2.44                     | 0.47              |
| 29:DC:56:GLN:C     | 29:DC:56:GLN:OE1   | 2.53                     | 0.47              |
| 30:DD:130:ALA:O    | 30:DD:131:LEU:HD12 | 2.15                     | 0.47              |
| 31:DE:23:VAL:HA    | 31:DE:186:GLY:H    | 1.79                     | 0.47              |
| 32:DF:109:GLY:CA   | 32:DF:112:MET:HB3  | 2.35                     | 0.47              |
| 32:DF:152:GLU:CB   | 32:DF:191:ARG:HD2  | 2.45                     | 0.47              |
| 33:DG:39:ILE:HD13  | 33:DG:157:ILE:HG23 | 1.97                     | 0.47              |
| 36:DN:3:THR:HG22   | 36:DN:5:VAL:CG1    | 2.44                     | 0.47              |
| 27:DA:1666:G:O3'   | 37:DO:6:THR:HG23   | 2.14                     | 0.47              |
| 38:DP:46:LYS:HG2   | 38:DP:52:GLU:CD    | 2.34                     | 0.47              |
| 41:DS:69:VAL:O     | 41:DS:72:ALA:HB3   | 2.14                     | 0.47              |
| 43:DU:50:ARG:CZ    | 44:DV:72:VAL:HG12  | 2.44                     | 0.47              |
| 36:DN:40:PRO:O     | 43:DU:64:ARG:HG2   | 2.15                     | 0.47              |
| 44:DV:12:TYR:CE2   | 44:DV:22:VAL:HG12  | 2.48                     | 0.47              |
| 1:AA:1302:U:OP1    | 13:AM:13:LYS:NZ    | 2.41                     | 0.47              |
| 1:AA:1412:C:H2'    | 1:AA:1413:A:H8     | 1.78                     | 0.47              |
| 1:AA:1399:C:C2     | 1:AA:1502:A:N6     | 2.83                     | 0.47              |
| 1:AA:622:A:C8      | 1:AA:623:C:C5      | 3.02                     | 0.47              |
| 1:AA:816:A:O2'     | 1:AA:817:C:P       | 2.73                     | 0.47              |
| 2:AB:187:LEU:CD2   | 2:AB:201:ILE:O     | 2.63                     | 0.47              |
| 3:AC:167:TRP:O     | 3:AC:168:ALA:HB2   | 2.13                     | 0.47              |
| 3:AC:41:GLY:O      | 3:AC:45:LYS:HG3    | 2.15                     | 0.47              |
| 4:AD:98:GLU:HA     | 4:AD:103:ASN:ND2   | 2.30                     | 0.47              |
| 4:AD:175:SER:OG    | 4:AD:184:LYS:HB2   | 2.14                     | 0.47              |
| 5:AE:53:LEU:H      | 5:AE:53:LEU:CD1    | 2.28                     | 0.47              |
| 7:AG:146:GLU:C     | 7:AG:148:ASN:N     | 2.68                     | 0.47              |
| 9:AI:114:TYR:N     | 9:AI:114:TYR:CD2   | 2.83                     | 0.47              |
| 10:AJ:95:GLU:CG    | 10:AJ:96:ILE:N     | 2.77                     | 0.47              |
| 12:AL:114:ARG:HH22 | 12:AL:121:LYS:CD   | 2.26                     | 0.47              |
| 14:AN:9:LYS:HG3    | 14:AN:12:ARG:CZ    | 2.45                     | 0.47              |
| 15:AO:76:GLU:C     | 15:AO:78:TYR:H     | 2.17                     | 0.47              |
| 19:AS:40:ILE:HG13  | 19:AS:69:HIS:O     | 2.15                     | 0.47              |
| 24:AX:2:G:N2       | 24:AX:72:A:H1'     | 2.30                     | 0.47              |
| 54:B5:45:VAL:O     | 54:B5:47:PRO:HD3   | 2.14                     | 0.47              |
| 27:BA:1033:U:C5'   | 27:BA:1034:G:OP1   | 2.61                     | 0.47              |
| 27:BA:113:G:H8     | 27:BA:113:G:OP2    | 1.97                     | 0.47              |
| 27:BA:1159:U:O2'   | 27:BA:1160:G:H5'   | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:30:G:O2'     | 27:BA:1214:A:N3    | 2.44                     | 0.47              |
| 27:BA:1249:U:H6    | 27:BA:1249:U:C5'   | 2.10                     | 0.47              |
| 27:BA:1848:A:C4    | 27:BA:1849:G:C8    | 3.03                     | 0.47              |
| 25:AY:75:A:O2'     | 27:BA:2394:C:N3    | 2.40                     | 0.47              |
| 27:BA:250:G:H2'    | 27:BA:251:A:H8     | 1.78                     | 0.47              |
| 27:BA:2554:U:H5'   | 27:BA:2554:U:H6    | 1.79                     | 0.47              |
| 27:BA:405:U:O2'    | 27:BA:406:G:H5'    | 2.15                     | 0.47              |
| 27:BA:638:G:O2'    | 27:BA:639:U:H5'    | 2.14                     | 0.47              |
| 30:BD:4:LYS:HE3    | 30:BD:21:PHE:HE1   | 1.80                     | 0.47              |
| 30:BD:26:LYS:O     | 30:BD:26:LYS:HG2   | 2.15                     | 0.47              |
| 33:BG:135:LEU:N    | 33:BG:135:LEU:HD12 | 2.30                     | 0.47              |
| 34:BH:25:LYS:HA    | 34:BH:33:LEU:O     | 2.14                     | 0.47              |
| 35:BI:117:GLU:HG3  | 35:BI:118:LYS:N    | 2.28                     | 0.47              |
| 35:BI:120:ILE:O    | 35:BI:121:LYS:CB   | 2.63                     | 0.47              |
| 38:BP:146:VAL:HG13 | 38:BP:147:LEU:H    | 1.76                     | 0.47              |
| 39:BQ:3:MET:HB2    | 39:BQ:4:PRO:HD2    | 1.96                     | 0.47              |
| 41:BS:93:LYS:O     | 41:BS:95:HIS:N     | 2.48                     | 0.47              |
| 46:BX:64:LYS:HE3   | 46:BX:64:LYS:HB2   | 1.61                     | 0.47              |
| 48:BZ:108:ALA:C    | 48:BZ:144:GLU:HG2  | 2.35                     | 0.47              |
| 39:BQ:108:GLY:CA   | 48:BZ:115:VAL:HG11 | 2.43                     | 0.47              |
| 48:BZ:18:ARG:NH1   | 48:BZ:81:ARG:NH2   | 2.61                     | 0.47              |
| 48:BZ:68:THR:HG22  | 48:BZ:89:VAL:CA    | 2.29                     | 0.47              |
| 1:CA:252:U:H2'     | 1:CA:253:U:H6      | 1.80                     | 0.47              |
| 1:CA:322:C:O2      | 1:CA:332:G:N2      | 2.46                     | 0.47              |
| 1:CA:397:A:C6      | 1:CA:548:G:N7      | 2.83                     | 0.47              |
| 1:CA:665:A:C8      | 1:CA:725:G:C2      | 3.03                     | 0.47              |
| 1:CA:96:U:H2'      | 1:CA:97:G:H8       | 1.77                     | 0.47              |
| 2:CB:56:ARG:NH1    | 2:CB:56:ARG:HG2    | 2.29                     | 0.47              |
| 2:CB:71:VAL:HG22   | 2:CB:93:VAL:HG22   | 1.96                     | 0.47              |
| 3:CC:84:ILE:O      | 3:CC:88:ARG:HG3    | 2.14                     | 0.47              |
| 5:CE:79:GLU:O      | 5:CE:80:ILE:HG23   | 2.15                     | 0.47              |
| 6:CF:97:PHE:HD2    | 18:CR:31:LEU:HD21  | 1.75                     | 0.47              |
| 7:CG:140:ASP:HA    | 7:CG:143:ARG:NH2   | 2.30                     | 0.47              |
| 12:CL:72:HIS:HD2   | 12:CL:74:LEU:HB2   | 1.79                     | 0.47              |
| 17:CQ:12:SER:HB3   | 17:CQ:20:THR:HB    | 1.96                     | 0.47              |
| 20:CT:53:LEU:HD12  | 20:CT:100:ILE:HB   | 1.96                     | 0.47              |
| 25:CY:29:G:C2      | 25:CY:40:C:O2      | 2.67                     | 0.47              |
| 27:DA:388:G:OP2    | 50:D1:25:LYS:HB2   | 2.14                     | 0.47              |
| 50:D1:6:GLU:OE1    | 50:D1:61:ARG:N     | 2.43                     | 0.47              |
| 56:D7:29:LYS:HG2   | 56:D7:33:ARG:NH2   | 2.29                     | 0.47              |
| 27:DA:973:A:O4'    | 27:DA:1188:U:C6    | 2.67                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:324:A:OP2   | 27:DA:1205:U:O4   | 2.33                     | 0.47              |
| 27:DA:1368:G:C2   | 27:DA:1369:G:C8   | 3.03                     | 0.47              |
| 27:DA:1952:A:N6   | 27:DA:1953:A:C6   | 2.83                     | 0.47              |
| 27:DA:1995:U:H2'  | 27:DA:1996:C:C5   | 2.49                     | 0.47              |
| 27:DA:209:C:H2'   | 27:DA:210:C:O4'   | 2.14                     | 0.47              |
| 27:DA:211:A:H2'   | 27:DA:212:G:H8    | 1.80                     | 0.47              |
| 27:DA:2396:G:N1   | 27:DA:2421:G:C6   | 2.82                     | 0.47              |
| 27:DA:2661:G:O2'  | 27:DA:2662:A:H5'  | 2.15                     | 0.47              |
| 27:DA:2822:G:OP2  | 40:DR:2:ARG:HD3   | 2.15                     | 0.47              |
| 27:DA:588:U:O2'   | 27:DA:589:C:O4'   | 2.32                     | 0.47              |
| 27:DA:682:G:H1    | 27:DA:795:C:H42   | 1.63                     | 0.47              |
| 27:DA:682:G:O6    | 27:DA:795:C:N4    | 2.46                     | 0.47              |
| 29:DC:19:VAL:HB   | 29:DC:22:ILE:HG12 | 1.95                     | 0.47              |
| 27:DA:2823:A:OP1  | 31:DE:113:PHE:HB3 | 2.15                     | 0.47              |
| 31:DE:151:TYR:O   | 31:DE:154:LYS:N   | 2.45                     | 0.47              |
| 31:DE:84:PHE:O    | 31:DE:84:PHE:CG   | 2.67                     | 0.47              |
| 32:DF:202:PHE:CG  | 32:DF:203:GLN:N   | 2.82                     | 0.47              |
| 32:DF:18:ARG:NH2  | 32:DF:20:LEU:HD13 | 2.26                     | 0.47              |
| 32:DF:84:VAL:C    | 32:DF:86:GLY:N    | 2.62                     | 0.47              |
| 36:DN:61:ARG:HG2  | 36:DN:61:ARG:H    | 1.54                     | 0.47              |
| 42:DT:53:ARG:HG2  | 42:DT:53:ARG:HH11 | 1.80                     | 0.47              |
| 43:DU:33:ARG:C    | 43:DU:35:ALA:H    | 2.18                     | 0.47              |
| 47:DY:26:LYS:NZ   | 47:DY:27:VAL:CG2  | 2.77                     | 0.47              |
| 47:DY:28:LYS:CB   | 47:DY:37:VAL:HB   | 2.43                     | 0.47              |
| 48:DZ:27:MET:HG2  | 48:DZ:34:ARG:O    | 2.15                     | 0.47              |
| 1:AA:1038:C:O5'   | 1:AA:1038:C:H6    | 1.98                     | 0.47              |
| 1:AA:1091:U:H2'   | 1:AA:1093:A:OP2   | 2.15                     | 0.47              |
| 1:AA:1228:C:H4'   | 13:AM:116:THR:O   | 2.15                     | 0.47              |
| 1:AA:1342:C:H1'   | 9:AI:124:GLN:HG2  | 1.96                     | 0.47              |
| 2:AB:114:ARG:O    | 2:AB:118:LEU:HG   | 2.15                     | 0.47              |
| 7:AG:115:ARG:HB2  | 7:AG:118:VAL:CG1  | 2.45                     | 0.47              |
| 8:AH:101:PRO:HG2  | 8:AH:133:LEU:CD1  | 2.39                     | 0.47              |
| 8:AH:12:ARG:HD3   | 8:AH:25:ASP:O     | 2.13                     | 0.47              |
| 8:AH:53:VAL:HG12  | 8:AH:56:LYS:HE2   | 1.96                     | 0.47              |
| 8:AH:50:ARG:HG2   | 8:AH:59:LEU:CD2   | 2.45                     | 0.47              |
| 10:AJ:63:PHE:HB3  | 14:AN:58:LYS:CA   | 2.43                     | 0.47              |
| 16:AP:6:LEU:HG    | 16:AP:19:ILE:HD13 | 1.97                     | 0.47              |
| 18:AR:34:TYR:HB3  | 18:AR:69:THR:HG22 | 1.96                     | 0.47              |
| 18:AR:37:VAL:O    | 18:AR:38:GLU:C    | 2.53                     | 0.47              |
| 19:AS:31:ILE:HG23 | 19:AS:49:ILE:HA   | 1.96                     | 0.47              |
| 1:AA:1286:A:C2    | 21:AU:22:ARG:NH2  | 2.83                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:B2:49:LYS:O    | 51:B2:52:ASP:HB2  | 2.15                     | 0.47              |
| 54:B5:49:CYS:O    | 54:B5:50:GLY:O    | 2.32                     | 0.47              |
| 27:BA:686:G:C6    | 56:B7:12:ARG:HA   | 2.50                     | 0.47              |
| 27:BA:1411:C:N4   | 27:BA:1412:A:N6   | 2.62                     | 0.47              |
| 27:BA:1613:G:O2'  | 56:B7:3:ARG:NE    | 2.47                     | 0.47              |
| 27:BA:1722:A:N6   | 27:BA:1740:G:C8   | 2.83                     | 0.47              |
| 27:BA:1904:G:H2'  | 27:BA:1905:C:O4'  | 2.15                     | 0.47              |
| 27:BA:2115:G:N2   | 27:BA:2119:A:N7   | 2.63                     | 0.47              |
| 27:BA:237:C:H2'   | 27:BA:238:C:C6    | 2.50                     | 0.47              |
| 27:BA:2416:C:O2'  | 27:BA:2417:C:H5'  | 2.14                     | 0.47              |
| 27:BA:2470:G:P    | 39:BQ:56:ARG:HH21 | 2.38                     | 0.47              |
| 27:BA:2771:C:H2'  | 27:BA:2772:C:H6   | 1.78                     | 0.47              |
| 27:BA:2782:G:N2   | 27:BA:2783:G:H1'  | 2.29                     | 0.47              |
| 27:BA:355:G:H2'   | 27:BA:356:G:O4'   | 2.14                     | 0.47              |
| 27:BA:684:G:O2'   | 27:BA:788:A:N7    | 2.47                     | 0.47              |
| 27:BA:81:G:H1     | 27:BA:105:C:N4    | 2.08                     | 0.47              |
| 27:BA:847:U:OP2   | 27:BA:928:G:O6    | 2.32                     | 0.47              |
| 28:BB:15:A:H4'    | 28:BB:16:G:OP2    | 2.15                     | 0.47              |
| 29:BC:197:GLU:O   | 29:BC:199:HIS:N   | 2.44                     | 0.47              |
| 29:BC:49:ILE:O    | 29:BC:51:PRO:CD   | 2.63                     | 0.47              |
| 30:BD:10:THR:O    | 30:BD:11:PRO:O    | 2.32                     | 0.47              |
| 27:BA:1826:G:O2'  | 30:BD:242:ARG:NH2 | 2.46                     | 0.47              |
| 31:BE:102:VAL:N   | 31:BE:170:LEU:O   | 2.48                     | 0.47              |
| 27:BA:2680:C:H4'  | 31:BE:188:VAL:O   | 2.15                     | 0.47              |
| 33:BG:18:GLU:O    | 33:BG:21:ARG:HB3  | 2.15                     | 0.47              |
| 36:BN:133:GLN:O   | 36:BN:134:ARG:CG  | 2.58                     | 0.47              |
| 37:BO:106:LEU:O   | 37:BO:108:GLU:N   | 2.47                     | 0.47              |
| 31:BE:52:LEU:CD1  | 42:BT:1:MET:CE    | 2.93                     | 0.47              |
| 42:BT:3:ARG:C     | 42:BT:5:ALA:N     | 2.63                     | 0.47              |
| 43:BU:76:TYR:CE1  | 43:BU:80:ILE:HD11 | 2.50                     | 0.47              |
| 43:BU:83:LEU:HD12 | 43:BU:88:ILE:HD11 | 1.96                     | 0.47              |
| 46:BX:21:PHE:O    | 46:BX:23:GLU:O    | 2.32                     | 0.47              |
| 27:BA:1599:C:H5'' | 46:BX:35:THR:HG22 | 1.96                     | 0.47              |
| 47:BY:14:LEU:O    | 47:BY:72:VAL:HA   | 2.15                     | 0.47              |
| 47:BY:26:LYS:HE3  | 47:BY:27:VAL:HG23 | 1.97                     | 0.47              |
| 1:CA:1315:U:H2'   | 1:CA:1316:G:C5'   | 2.45                     | 0.47              |
| 1:CA:1404:C:O2    | 1:CA:1519:A:O2'   | 2.32                     | 0.47              |
| 1:CA:321:A:H4'    | 1:CA:1436:U:C4'   | 2.44                     | 0.47              |
| 1:CA:391:G:C6     | 1:CA:392:G:N7     | 2.83                     | 0.47              |
| 1:CA:659:U:C4     | 1:CA:660:G:N7     | 2.83                     | 0.47              |
| 1:CA:814:A:N7     | 1:CA:816:A:C4     | 2.83                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CB:85:ALA:HB3    | 2:CB:92:TYR:HD2   | 1.78                     | 0.47              |
| 4:CD:187:ARG:NH1   | 4:CD:187:ARG:HG2  | 2.29                     | 0.47              |
| 9:CI:19:LEU:CD2    | 9:CI:61:ALA:HB2   | 2.44                     | 0.47              |
| 10:CJ:78:ASN:ND2   | 10:CJ:80:LYS:H    | 2.13                     | 0.47              |
| 15:CO:81:LEU:HD11  | 15:CO:85:LEU:HD12 | 1.95                     | 0.47              |
| 17:CQ:64:PRO:HB3   | 17:CQ:70:ARG:HE   | 1.78                     | 0.47              |
| 19:CS:22:LEU:O     | 19:CS:26:GLY:HA2  | 2.15                     | 0.47              |
| 19:CS:39:THR:HG22  | 19:CS:40:ILE:N    | 2.29                     | 0.47              |
| 22:CV:2:A:H2'      | 22:CV:3:A:H8      | 1.80                     | 0.47              |
| 24:CX:59:A:O2'     | 24:CX:60:U:H5'    | 2.15                     | 0.47              |
| 50:D1:57:GLU:O     | 50:D1:58:ILE:O    | 2.33                     | 0.47              |
| 50:D1:75:GLU:HA    | 50:D1:75:GLU:OE2  | 2.15                     | 0.47              |
| 27:DA:1209:G:HO2'  | 27:DA:1237:A:H61  | 1.61                     | 0.47              |
| 27:DA:1844:C:C4    | 27:DA:1845:G:N7   | 2.82                     | 0.47              |
| 27:DA:2083:G:H2'   | 27:DA:2084:C:H6   | 1.80                     | 0.47              |
| 27:DA:2249:U:H4'   | 27:DA:2250:G:OP2  | 2.13                     | 0.47              |
| 27:DA:2253:G:H2'   | 27:DA:2254:C:H6   | 1.80                     | 0.47              |
| 27:DA:2684:U:C4    | 27:DA:2685:G:N7   | 2.83                     | 0.47              |
| 27:DA:2803:C:OP1   | 27:DA:2803:C:H4'  | 2.13                     | 0.47              |
| 27:DA:2839:G:C6    | 27:DA:2840:C:N3   | 2.83                     | 0.47              |
| 27:DA:2891:G:O5'   | 27:DA:2891:G:H8   | 1.96                     | 0.47              |
| 27:DA:501:A:H2'    | 27:DA:502:A:C8    | 2.49                     | 0.47              |
| 27:DA:501:A:H2'    | 27:DA:502:A:H8    | 1.79                     | 0.47              |
| 27:DA:71:A:C8      | 27:DA:71:A:H5'    | 2.50                     | 0.47              |
| 30:DD:208:LYS:HG3  | 30:DD:210:GLY:N   | 2.29                     | 0.47              |
| 30:DD:26:LYS:HZ2   | 30:DD:82:ILE:HB   | 1.79                     | 0.47              |
| 31:DE:14:ILE:HG13  | 31:DE:14:ILE:O    | 2.15                     | 0.47              |
| 31:DE:179:GLU:CA   | 31:DE:179:GLU:OE1 | 2.62                     | 0.47              |
| 31:DE:61:ARG:HD2   | 31:DE:62:PRO:HD3  | 1.97                     | 0.47              |
| 38:DP:101:VAL:HG23 | 38:DP:102:ARG:N   | 2.30                     | 0.47              |
| 39:DQ:16:ARG:CG    | 39:DQ:17:LEU:N    | 2.71                     | 0.47              |
| 39:DQ:42:ILE:H     | 39:DQ:42:ILE:CD1  | 2.23                     | 0.47              |
| 41:DS:14:VAL:O     | 41:DS:16:ASN:N    | 2.47                     | 0.47              |
| 42:DT:132:LYS:C    | 42:DT:134:GLU:N   | 2.68                     | 0.47              |
| 42:DT:35:LYS:HG3   | 42:DT:36:GLU:N    | 2.30                     | 0.47              |
| 42:DT:51:ARG:CD    | 42:DT:62:THR:HG23 | 2.32                     | 0.47              |
| 42:DT:64:ARG:HA    | 42:DT:72:VAL:O    | 2.15                     | 0.47              |
| 1:AA:1157:A:C4'    | 1:AA:1158:C:O5'   | 2.54                     | 0.47              |
| 1:AA:1381:U:H2'    | 1:AA:1381:U:O2    | 2.13                     | 0.47              |
| 1:AA:1420:C:H2'    | 1:AA:1421:G:H8    | 1.80                     | 0.47              |
| 1:AA:306:G:H2'     | 1:AA:307:C:C6     | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:30:U:H4'     | 1:AA:31:G:OP1     | 2.10                     | 0.47              |
| 2:AB:96:ARG:O     | 2:AB:97:TRP:C     | 2.53                     | 0.47              |
| 3:AC:41:GLY:C     | 3:AC:45:LYS:NZ    | 2.68                     | 0.47              |
| 4:AD:28:SER:HB2   | 4:AD:30:LYS:HG2   | 1.97                     | 0.47              |
| 6:AF:44:GLY:O     | 6:AF:59:TYR:HA    | 2.15                     | 0.47              |
| 6:AF:65:VAL:HG23  | 6:AF:66:GLU:N     | 2.29                     | 0.47              |
| 7:AG:23:VAL:O     | 7:AG:27:ILE:HG13  | 2.15                     | 0.47              |
| 8:AH:56:LYS:O     | 8:AH:58:TYR:HD1   | 1.97                     | 0.47              |
| 8:AH:57:PRO:O     | 8:AH:58:TYR:CD1   | 2.67                     | 0.47              |
| 10:AJ:34:VAL:HG22 | 10:AJ:74:ILE:HA   | 1.97                     | 0.47              |
| 11:AK:95:ILE:O    | 11:AK:98:LEU:N    | 2.48                     | 0.47              |
| 13:AM:116:THR:O   | 13:AM:117:VAL:CB  | 2.63                     | 0.47              |
| 14:AN:27:CYS:C    | 14:AN:29:ARG:H    | 2.12                     | 0.47              |
| 15:AO:16:ALA:HB1  | 15:AO:21:ASP:HB3  | 1.97                     | 0.47              |
| 17:AQ:63:ARG:HG2  | 17:AQ:64:PRO:CD   | 2.43                     | 0.47              |
| 18:AR:40:LEU:C    | 18:AR:42:ARG:N    | 2.67                     | 0.47              |
| 23:AW:72:G:H5'    | 23:AW:73:C:OP1    | 2.13                     | 0.47              |
| 24:AX:15:G:N2     | 24:AX:21:A:N3     | 2.62                     | 0.47              |
| 24:AX:51:C:H2'    | 24:AX:52:G:H8     | 1.79                     | 0.47              |
| 25:AY:23:G:H2'    | 25:AY:24:C:C6     | 2.50                     | 0.47              |
| 50:B1:57:GLU:C    | 50:B1:58:ILE:HG23 | 2.36                     | 0.47              |
| 53:B4:41:ILE:O    | 53:B4:59:VAL:N    | 2.46                     | 0.47              |
| 57:B8:14:VAL:CG2  | 57:B8:22:VAL:HG12 | 2.45                     | 0.47              |
| 57:B8:25:MET:O    | 57:B8:47:LYS:NZ   | 2.45                     | 0.47              |
| 58:B9:2:LYS:O     | 58:B9:35:ARG:N    | 2.48                     | 0.47              |
| 27:BA:1167:U:C2   | 27:BA:1183:G:N2   | 2.83                     | 0.47              |
| 27:BA:1491:G:OP1  | 27:BA:1494:A:N6   | 2.48                     | 0.47              |
| 27:BA:413:C:H4'   | 27:BA:1880:C:O2'  | 2.14                     | 0.47              |
| 27:BA:2228:G:OP1  | 30:BD:261:LYS:HE3 | 2.14                     | 0.47              |
| 27:BA:2259:G:O4'  | 27:BA:2427:C:H2'  | 2.15                     | 0.47              |
| 27:BA:2586:C:O2'  | 27:BA:2587:A:H5'  | 2.15                     | 0.47              |
| 27:BA:2716:U:H2'  | 27:BA:2717:G:H8   | 1.79                     | 0.47              |
| 27:BA:2790:A:H2'  | 27:BA:2791:C:H5'' | 1.96                     | 0.47              |
| 27:BA:854:G:C2    | 27:BA:855:G:C5    | 3.03                     | 0.47              |
| 27:BA:969:U:O3'   | 52:B3:14:GLY:HA2  | 2.15                     | 0.47              |
| 28:BB:82:G:H2'    | 28:BB:83:G:O4'    | 2.15                     | 0.47              |
| 30:BD:75:ILE:HG22 | 30:BD:76:PRO:HD2  | 1.97                     | 0.47              |
| 33:BG:88:ILE:HG13 | 33:BG:89:GLY:N    | 2.27                     | 0.47              |
| 37:BO:113:LYS:O   | 37:BO:114:ILE:C   | 2.50                     | 0.47              |
| 40:BR:10:LEU:HA   | 40:BR:17:ARG:CD   | 2.40                     | 0.47              |
| 42:BT:57:PHE:O    | 42:BT:58:ASN:C    | 2.52                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BU:101:ARG:O    | 43:BU:102:GLU:CB   | 2.62                     | 0.47              |
| 47:BY:28:LYS:HG3   | 47:BY:30:VAL:HG23  | 1.97                     | 0.47              |
| 48:BZ:36:VAL:HG23  | 48:BZ:37:TYR:N     | 2.28                     | 0.47              |
| 1:CA:1063:C:H3'    | 1:CA:1063:C:H6     | 1.79                     | 0.47              |
| 1:CA:1239:A:H4'    | 1:CA:1240:U:O5'    | 2.15                     | 0.47              |
| 1:CA:1272:G:H8     | 1:CA:1272:G:H5''   | 1.80                     | 0.47              |
| 1:CA:142:G:H1      | 1:CA:221:C:N4      | 2.08                     | 0.47              |
| 1:CA:1480:G:C5     | 1:CA:1481:U:C5     | 3.03                     | 0.47              |
| 1:CA:393:A:OP2     | 16:CP:12:LYS:HE2   | 2.15                     | 0.47              |
| 1:CA:731:G:N2      | 1:CA:732:C:O2      | 2.48                     | 0.47              |
| 3:CC:19:GLU:O      | 3:CC:20:SER:HB2    | 2.15                     | 0.47              |
| 4:CD:23:GLY:O      | 4:CD:25:ARG:N      | 2.48                     | 0.47              |
| 5:CE:55:VAL:O      | 5:CE:58:ALA:HB3    | 2.14                     | 0.47              |
| 7:CG:116:ALA:O     | 7:CG:119:ARG:HB2   | 2.15                     | 0.47              |
| 8:CH:29:SER:O      | 8:CH:30:ARG:C      | 2.52                     | 0.47              |
| 8:CH:63:LEU:H      | 8:CH:63:LEU:HD22   | 1.79                     | 0.47              |
| 9:CI:27:THR:HG23   | 9:CI:31:GLN:C      | 2.35                     | 0.47              |
| 9:CI:52:ALA:HB3    | 9:CI:95:LYS:CE     | 2.44                     | 0.47              |
| 10:CJ:34:VAL:HG13  | 10:CJ:73:ASP:O     | 2.14                     | 0.47              |
| 1:CA:975:A:N6      | 10:CJ:48:THR:HB    | 2.20                     | 0.47              |
| 11:CK:29:ILE:CD1   | 11:CK:44:SER:HB3   | 2.43                     | 0.47              |
| 13:CM:69:GLU:OE1   | 13:CM:72:ALA:CB    | 2.60                     | 0.47              |
| 16:CP:72:ARG:HH21  | 16:CP:73:LEU:HD21  | 1.80                     | 0.47              |
| 20:CT:87:LYS:C     | 20:CT:89:ARG:H     | 2.17                     | 0.47              |
| 1:CA:530:G:O2'     | 23:CW:34:U:H4'     | 2.14                     | 0.47              |
| 25:CY:68:C:H3'     | 25:CY:69:C:H5''    | 1.97                     | 0.47              |
| 49:D0:51:VAL:N     | 49:D0:62:LEU:HD12  | 2.30                     | 0.47              |
| 50:D1:69:LYS:HA    | 50:D1:72:GLU:HB3   | 1.95                     | 0.47              |
| 55:D6:22:ALA:C     | 55:D6:23:THR:HG23  | 2.35                     | 0.47              |
| 27:DA:1385:G:O2'   | 27:DA:1396:U:H6    | 1.98                     | 0.47              |
| 27:DA:1395:A:OP1   | 27:DA:1603:A:OP1   | 2.32                     | 0.47              |
| 27:DA:1927:A:H8    | 27:DA:1927:A:OP1   | 1.98                     | 0.47              |
| 27:DA:1833:U:O2'   | 27:DA:1969:A:N1    | 2.44                     | 0.47              |
| 27:DA:2019:A:C6    | 27:DA:2020:A:C5    | 3.03                     | 0.47              |
| 27:DA:2055:C:H2'   | 27:DA:2055:C:O2    | 2.13                     | 0.47              |
| 27:DA:2078:C:H2'   | 27:DA:2079:U:C6    | 2.50                     | 0.47              |
| 27:DA:2121:G:C2    | 27:DA:2122:U:C2    | 3.03                     | 0.47              |
| 27:DA:2291:U:H5''  | 27:DA:2380:C:O2'   | 2.15                     | 0.47              |
| 27:DA:2674:G:H2'   | 27:DA:2675:A:C8    | 2.50                     | 0.47              |
| 27:DA:271(W):G:H5' | 27:DA:271(X):G:OP2 | 2.15                     | 0.47              |
| 27:DA:2758:A:C3'   | 27:DA:2759:G:H5''  | 2.45                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:301:G:N2     | 27:DA:316:C:N3     | 2.47                     | 0.47              |
| 27:DA:52:A:N3      | 27:DA:53:A:C8      | 2.83                     | 0.47              |
| 27:DA:763:G:C2     | 27:DA:765:G:H1'    | 2.50                     | 0.47              |
| 27:DA:90:U:O2      | 27:DA:90:U:C2'     | 2.63                     | 0.47              |
| 31:DE:129:HIS:O    | 31:DE:130:GLY:O    | 2.32                     | 0.47              |
| 31:DE:127:ASP:HA   | 31:DE:135:HIS:ND1  | 2.29                     | 0.47              |
| 31:DE:199:ARG:HB3  | 31:DE:200:GLU:H    | 1.39                     | 0.47              |
| 32:DF:3:GLU:O      | 32:DF:4:VAL:C      | 2.53                     | 0.47              |
| 34:DH:127:GLU:C    | 34:DH:129:THR:H    | 2.18                     | 0.47              |
| 35:DI:37:VAL:CG1   | 35:DI:38:LEU:N     | 2.75                     | 0.47              |
| 35:DI:94:ALA:CB    | 35:DI:114:LEU:HD11 | 2.45                     | 0.47              |
| 27:DA:558:G:H4'    | 36:DN:44:PRO:O     | 2.14                     | 0.47              |
| 27:DA:1665:A:H1'   | 37:DO:1:MET:CE     | 2.45                     | 0.47              |
| 37:DO:20:MET:CG    | 37:DO:21:CYS:N     | 2.78                     | 0.47              |
| 37:DO:16:ALA:CB    | 37:DO:52:VAL:HG11  | 2.43                     | 0.47              |
| 27:DA:1011:G:OP1   | 43:DU:77:SER:CB    | 2.62                     | 0.47              |
| 43:DU:90:VAL:C     | 43:DU:92:ARG:H     | 2.18                     | 0.47              |
| 45:DW:105:VAL:HG12 | 45:DW:107:LEU:CD1  | 2.45                     | 0.47              |
| 45:DW:60:ASN:HD22  | 45:DW:60:ASN:N     | 2.12                     | 0.47              |
| 46:DX:12:VAL:HB    | 46:DX:17:ALA:CB    | 2.45                     | 0.47              |
| 46:DX:26:TYR:CE1   | 46:DX:89:ILE:HD12  | 2.50                     | 0.47              |
| 47:DY:90:LEU:HD12  | 47:DY:91:GLU:H     | 1.80                     | 0.47              |
| 1:AA:1206:G:H2'    | 1:AA:1207:G:C5'    | 2.42                     | 0.47              |
| 1:AA:1246:C:H2'    | 1:AA:1246:C:O2     | 2.14                     | 0.47              |
| 1:AA:1500:A:H5''   | 1:AA:1508:G:H5''   | 1.96                     | 0.47              |
| 1:AA:370:C:H2'     | 1:AA:371:G:H8      | 1.79                     | 0.47              |
| 1:AA:60:A:OP1      | 1:AA:111:G:N2      | 2.47                     | 0.47              |
| 1:AA:652:U:O2'     | 1:AA:653:A:O5'     | 2.33                     | 0.47              |
| 1:AA:976:G:N7      | 1:AA:1358:U:C2     | 2.82                     | 0.47              |
| 2:AB:71:VAL:HB     | 2:AB:164:VAL:HG22  | 1.96                     | 0.47              |
| 3:AC:42:LEU:HA     | 3:AC:45:LYS:CG     | 2.45                     | 0.47              |
| 5:AE:133:TYR:N     | 5:AE:133:TYR:CD1   | 2.81                     | 0.47              |
| 7:AG:45:ASP:HB3    | 7:AG:117:ALA:HB1   | 1.97                     | 0.47              |
| 9:AI:96:LEU:HG     | 9:AI:102:LEU:HB2   | 1.96                     | 0.47              |
| 12:AL:38:ARG:NH2   | 12:AL:54:LYS:NZ    | 2.62                     | 0.47              |
| 13:AM:91:ARG:HB3   | 13:AM:98:VAL:HG13  | 1.97                     | 0.47              |
| 1:AA:1060:C:P      | 14:AN:45:ARG:NH2   | 2.88                     | 0.47              |
| 17:AQ:22:LEU:CD1   | 17:AQ:41:LYS:HG2   | 2.43                     | 0.47              |
| 17:AQ:67:LYS:HA    | 17:AQ:70:ARG:HH12  | 1.79                     | 0.47              |
| 18:AR:82:THR:HG22  | 18:AR:83:GLU:N     | 2.30                     | 0.47              |
| 49:B0:51:VAL:HG21  | 49:B0:79:VAL:O     | 2.15                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 55:B6:15:GLU:OE1   | 55:B6:41:PRO:HB3  | 2.15                     | 0.47              |
| 55:B6:51:GLU:O     | 55:B6:52:VAL:CG2  | 2.62                     | 0.47              |
| 27:BA:119:A:O2'    | 27:BA:120:U:O5'   | 2.28                     | 0.47              |
| 27:BA:127:A:H5''   | 27:BA:128:C:C6    | 2.50                     | 0.47              |
| 27:BA:1612:C:N3    | 27:BA:1620:G:C2   | 2.82                     | 0.47              |
| 27:BA:1987:G:H2'   | 27:BA:1988:C:C6   | 2.49                     | 0.47              |
| 27:BA:2087:G:O2'   | 27:BA:2088:G:H5'  | 2.15                     | 0.47              |
| 27:BA:2637:U:H5'   | 31:BE:44:TYR:CD1  | 2.49                     | 0.47              |
| 27:BA:2644:G:H2'   | 27:BA:2645:G:C8   | 2.50                     | 0.47              |
| 27:BA:27:G:H1'     | 27:BA:513:A:H62   | 1.80                     | 0.47              |
| 27:BA:2842:G:C2    | 27:BA:2876:G:C2   | 3.02                     | 0.47              |
| 27:BA:56:A:O2'     | 27:BA:57:C:C5'    | 2.59                     | 0.47              |
| 27:BA:577:G:H5'    | 27:BA:2502:G:C2   | 2.50                     | 0.47              |
| 27:BA:660:G:O3'    | 32:BF:38:ARG:NH2  | 2.47                     | 0.47              |
| 27:BA:675:A:C6     | 27:BA:676:A:C6    | 3.03                     | 0.47              |
| 27:BA:689:A:N3     | 27:BA:779:U:O2'   | 2.42                     | 0.47              |
| 27:BA:904:C:H2'    | 27:BA:905:U:H5'   | 1.96                     | 0.47              |
| 31:BE:154:LYS:O    | 31:BE:156:MET:HG3 | 2.15                     | 0.47              |
| 40:BR:20:LEU:C     | 40:BR:22:ARG:N    | 2.68                     | 0.47              |
| 41:BS:101:LEU:HD22 | 41:BS:102:ALA:O   | 2.15                     | 0.47              |
| 41:BS:66:ALA:O     | 41:BS:69:VAL:HG13 | 2.14                     | 0.47              |
| 43:BU:106:PHE:O    | 43:BU:107:ALA:C   | 2.52                     | 0.47              |
| 43:BU:47:TYR:O     | 43:BU:51:LYS:HG2  | 2.15                     | 0.47              |
| 44:BV:47:VAL:O     | 44:BV:47:VAL:HG23 | 2.15                     | 0.47              |
| 1:CA:1472:U:H2'    | 1:CA:1473:A:C8    | 2.49                     | 0.47              |
| 1:CA:153:C:H2'     | 1:CA:154:C:H6     | 1.80                     | 0.47              |
| 1:CA:285:G:N1      | 1:CA:286:G:C5     | 2.82                     | 0.47              |
| 1:CA:426:G:OP1     | 4:CD:36:ARG:NE    | 2.47                     | 0.47              |
| 1:CA:754:C:C2'     | 1:CA:754:C:O2     | 2.54                     | 0.47              |
| 3:CC:11:ARG:HB3    | 3:CC:15:THR:HB    | 1.97                     | 0.47              |
| 3:CC:59:ARG:HA     | 3:CC:63:ASN:O     | 2.15                     | 0.47              |
| 4:CD:148:VAL:HG21  | 4:CD:181:MET:HE2  | 1.96                     | 0.47              |
| 4:CD:91:SER:O      | 4:CD:94:LEU:N     | 2.48                     | 0.47              |
| 5:CE:52:PRO:HD2    | 5:CE:53:LEU:HD12  | 1.96                     | 0.47              |
| 7:CG:139:GLU:C     | 7:CG:141:VAL:N    | 2.64                     | 0.47              |
| 9:CI:24:GLY:O      | 9:CI:26:VAL:HG23  | 2.15                     | 0.47              |
| 10:CJ:3:LYS:O      | 10:CJ:100:THR:HA  | 2.14                     | 0.47              |
| 10:CJ:97:GLU:C     | 10:CJ:98:ILE:HD12 | 2.34                     | 0.47              |
| 12:CL:34:CYS:HA    | 12:CL:55:VAL:HG22 | 1.95                     | 0.47              |
| 15:CO:2:PRO:O      | 15:CO:38:ARG:NE   | 2.44                     | 0.47              |
| 1:CA:624:C:O2'     | 16:CP:10:GLY:HA2  | 2.14                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:CS:12:ASP:HB3   | 19:CS:14:HIS:CE1  | 2.50                     | 0.47              |
| 23:CW:10:G:H1      | 23:CW:25:A:H1'    | 1.80                     | 0.47              |
| 23:CW:10:G:N2      | 23:CW:25:A:H1'    | 2.30                     | 0.47              |
| 24:CX:5:G:H1       | 24:CX:68:C:H42    | 1.63                     | 0.47              |
| 25:CY:67:C:H2'     | 25:CY:68:C:C6     | 2.49                     | 0.47              |
| 52:D3:11:SER:HA    | 52:D3:12:PRO:HD3  | 1.61                     | 0.47              |
| 54:D5:45:VAL:HG22  | 54:D5:51:TYR:HD2  | 1.79                     | 0.47              |
| 27:DA:459:U:OP1    | 56:D7:39:ARG:HA   | 2.13                     | 0.47              |
| 57:D8:37:SER:OG    | 57:D8:40:GLU:N    | 2.47                     | 0.47              |
| 57:D8:7:HIS:HD1    | 57:D8:7:HIS:C     | 2.18                     | 0.47              |
| 27:DA:1024:G:OP2   | 27:DA:1025:G:H3'  | 2.15                     | 0.47              |
| 27:DA:1170:G:N2    | 27:DA:1179:C:H42  | 2.12                     | 0.47              |
| 27:DA:1291:C:O2'   | 27:DA:1292:U:C5'  | 2.63                     | 0.47              |
| 27:DA:1427:A:O2'   | 27:DA:1428:C:OP2  | 2.29                     | 0.47              |
| 27:DA:1658:C:O5'   | 27:DA:1658:C:H6   | 1.96                     | 0.47              |
| 27:DA:1764:G:H21   | 27:DA:1765:C:H1'  | 1.80                     | 0.47              |
| 27:DA:1842:G:C6    | 27:DA:1843:C:N3   | 2.83                     | 0.47              |
| 27:DA:203:C:O5'    | 27:DA:204:A:H5''  | 2.15                     | 0.47              |
| 27:DA:208:C:O2'    | 27:DA:209:C:H5'   | 2.15                     | 0.47              |
| 27:DA:2468:G:H22   | 27:DA:2481:G:C2'  | 2.27                     | 0.47              |
| 27:DA:1662:C:O2'   | 27:DA:2687:U:OP1  | 2.30                     | 0.47              |
| 27:DA:2788:C:O2'   | 27:DA:2809:A:N3   | 2.43                     | 0.47              |
| 27:DA:286:C:H2'    | 27:DA:287:C:C5'   | 2.45                     | 0.47              |
| 27:DA:30:G:O2'     | 27:DA:31:C:H5'    | 2.14                     | 0.47              |
| 27:DA:484:C:O5'    | 27:DA:484:C:H6    | 1.97                     | 0.47              |
| 27:DA:682:G:H1     | 27:DA:795:C:N4    | 2.12                     | 0.47              |
| 27:DA:7:G:H1       | 27:DA:2896:C:H42  | 1.62                     | 0.47              |
| 27:DA:81:G:H21     | 47:DY:2:ARG:NH2   | 2.13                     | 0.47              |
| 30:DD:193:VAL:HG22 | 30:DD:194:GLY:N   | 2.30                     | 0.47              |
| 30:DD:221:VAL:HG23 | 30:DD:226:MET:HE2 | 1.96                     | 0.47              |
| 32:DF:50:SER:HB2   | 32:DF:94:PRO:HG3  | 1.96                     | 0.47              |
| 33:DG:70:VAL:HA    | 33:DG:89:GLY:O    | 2.15                     | 0.47              |
| 36:DN:118:LYS:C    | 36:DN:120:LEU:N   | 2.66                     | 0.47              |
| 27:DA:587:C:H2'    | 38:DP:33:ARG:NH2  | 2.30                     | 0.47              |
| 39:DQ:35:VAL:HG23  | 39:DQ:101:ARG:O   | 2.15                     | 0.47              |
| 40:DR:2:ARG:HB2    | 40:DR:3:HIS:H     | 1.48                     | 0.47              |
| 42:DT:11:GLU:H     | 42:DT:11:GLU:CD   | 2.16                     | 0.47              |
| 43:DU:59:ARG:O     | 43:DU:62:ILE:N    | 2.42                     | 0.47              |
| 46:DX:66:LEU:C     | 46:DX:66:LEU:HD23 | 2.35                     | 0.47              |
| 47:DY:46:LYS:HB3   | 47:DY:47:LYS:H    | 1.54                     | 0.47              |
| 1:AA:1026:G:H2'    | 1:AA:1026:G:N3    | 2.28                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:105:G:C6      | 1:AA:106:C:N3     | 2.83                     | 0.47              |
| 1:AA:1118:C:O2'    | 1:AA:1119:C:H5'   | 2.15                     | 0.47              |
| 1:AA:1286:A:H2     | 21:AU:22:ARG:NH2  | 2.13                     | 0.47              |
| 1:AA:1459:C:O2'    | 1:AA:1460:A:H5'   | 2.15                     | 0.47              |
| 1:AA:169:C:C2'     | 1:AA:170:U:H5'    | 2.45                     | 0.47              |
| 1:AA:659:U:P       | 15:AO:8:LYS:HE2   | 2.54                     | 0.47              |
| 1:AA:749:C:H2'     | 1:AA:750:G:H8     | 1.79                     | 0.47              |
| 2:AB:48:MET:O      | 2:AB:49:GLU:C     | 2.52                     | 0.47              |
| 4:AD:119:GLN:NE2   | 4:AD:123:HIS:CD2  | 2.79                     | 0.47              |
| 4:AD:187:ARG:HH11  | 4:AD:187:ARG:HG2  | 1.80                     | 0.47              |
| 5:AE:33:VAL:HG22   | 5:AE:42:GLY:O     | 2.15                     | 0.47              |
| 7:AG:64:GLN:O      | 7:AG:68:ASN:HB2   | 2.15                     | 0.47              |
| 7:AG:70:LYS:HB3    | 7:AG:96:GLN:CG    | 2.44                     | 0.47              |
| 8:AH:74:PRO:CG     | 8:AH:75:ARG:H     | 2.28                     | 0.47              |
| 9:AI:45:ALA:C      | 9:AI:47:LEU:H     | 2.16                     | 0.47              |
| 11:AK:93:GLN:HA    | 11:AK:93:GLN:OE1  | 2.15                     | 0.47              |
| 12:AL:63:VAL:HG21  | 12:AL:95:TYR:CD1  | 2.50                     | 0.47              |
| 1:AA:1202:G:C4     | 14:AN:42:ILE:HD13 | 2.50                     | 0.47              |
| 15:AO:62:GLN:O     | 15:AO:65:ARG:HB2  | 2.15                     | 0.47              |
| 18:AR:33:ASP:OD2   | 18:AR:35:ARG:N    | 2.46                     | 0.47              |
| 1:AA:1305:G:P      | 21:AU:2:GLY:N     | 2.87                     | 0.47              |
| 25:AY:32:U:O2'     | 25:AY:35:G:N7     | 2.39                     | 0.47              |
| 27:BA:978:G:O4'    | 27:BA:1001:A:C2   | 2.68                     | 0.47              |
| 27:BA:1213:A:C2    | 27:BA:1214:A:C4   | 3.02                     | 0.47              |
| 27:BA:1310:G:O2'   | 27:BA:1311:G:H5'  | 2.15                     | 0.47              |
| 27:BA:1332:G:H22   | 27:BA:1609:A:H2'  | 1.79                     | 0.47              |
| 27:BA:140:G:N3     | 27:BA:142:A:N1    | 2.63                     | 0.47              |
| 27:BA:1465:G:C4    | 27:BA:1466:G:C8   | 3.03                     | 0.47              |
| 27:BA:1912:A:H5'   | 27:BA:1918:A:N1   | 2.28                     | 0.47              |
| 27:BA:2533:A:H3'   | 27:BA:2534:A:H5'' | 1.96                     | 0.47              |
| 27:BA:2563:U:H2'   | 27:BA:2564:A:H3'  | 1.96                     | 0.47              |
| 27:BA:2642:G:C6    | 27:BA:2643:G:C5   | 3.03                     | 0.47              |
| 27:BA:2692:C:H2'   | 27:BA:2693:A:C8   | 2.50                     | 0.47              |
| 27:BA:2773:C:H2'   | 27:BA:2774:C:C6   | 2.43                     | 0.47              |
| 27:BA:2834:G:C4    | 27:BA:2879:C:N4   | 2.83                     | 0.47              |
| 27:BA:295:G:N1     | 27:BA:296:C:C4    | 2.83                     | 0.47              |
| 27:BA:339:U:C2'    | 27:BA:340:A:H5'   | 2.45                     | 0.47              |
| 27:BA:272(E):G:C6  | 27:BA:364:C:N4    | 2.83                     | 0.47              |
| 27:BA:614(C):A:H4' | 27:BA:615:G:OP1   | 2.15                     | 0.47              |
| 30:BD:24:ILE:O     | 30:BD:26:LYS:HD3  | 2.14                     | 0.47              |
| 31:BE:26:ILE:HB    | 31:BE:182:LEU:HB3 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:BE:3:GLY:HA3  | 31:BE:81:ILE:CG2  | 2.45                     | 0.47              |
| 34:BH:82:GLY:O   | 34:BH:83:TYR:O    | 2.32                     | 0.47              |
| 36:BN:30:ILE:CG2 | 36:BN:52:VAL:HG11 | 2.35                     | 0.47              |
| 37:BO:97:ARG:C   | 37:BO:98:VAL:HG12 | 2.35                     | 0.47              |
| 38:BP:63:PRO:C   | 38:BP:65:ARG:N    | 2.69                     | 0.47              |
| 39:BQ:39:PRO:HD3 | 39:BQ:99:PRO:HG3  | 1.96                     | 0.47              |
| 47:BY:42:VAL:O   | 47:BY:65:ALA:HB3  | 2.15                     | 0.47              |
| 47:BY:79:CYS:O   | 47:BY:80:GLY:C    | 2.53                     | 0.47              |
| 48:BZ:16:ALA:O   | 48:BZ:19:ARG:N    | 2.48                     | 0.47              |
| 1:CA:1058:G:H2'  | 1:CA:1059:C:O4'   | 2.15                     | 0.47              |
| 1:CA:182:U:H2'   | 1:CA:182:U:O2     | 2.14                     | 0.47              |
| 1:CA:274:A:O2'   | 1:CA:275:G:H8     | 1.96                     | 0.47              |
| 1:CA:50:A:H1'    | 1:CA:52:G:C8      | 2.49                     | 0.47              |
| 1:CA:699:C:C2'   | 1:CA:700:G:H5'    | 2.44                     | 0.47              |
| 1:CA:962:C:H2'   | 1:CA:963:G:H8     | 1.79                     | 0.47              |
| 1:CA:973:G:OP1   | 10:CJ:57:LYS:HD3  | 2.15                     | 0.47              |
| 1:CA:978:A:C5'   | 1:CA:978:A:C8     | 2.98                     | 0.47              |
| 2:CB:87:ARG:NE   | 2:CB:233:SER:HB2  | 2.30                     | 0.47              |
| 4:CD:13:ARG:O    | 4:CD:16:GLY:N     | 2.44                     | 0.47              |
| 4:CD:64:LEU:O    | 4:CD:65:ARG:C     | 2.54                     | 0.47              |
| 6:CF:30:LEU:C    | 6:CF:35:ALA:HB3   | 2.35                     | 0.47              |
| 7:CG:143:ARG:HB2 | 7:CG:143:ARG:NH1  | 2.30                     | 0.47              |
| 7:CG:26:PHE:CD2  | 7:CG:62:PHE:HE1   | 2.33                     | 0.47              |
| 9:CI:112:LYS:NZ  | 9:CI:113:LYS:O    | 2.48                     | 0.47              |
| 12:CL:33:VAL:C   | 12:CL:55:VAL:HG13 | 2.35                     | 0.47              |
| 12:CL:5:ASN:CB   | 17:CQ:34:LYS:HZ3  | 2.27                     | 0.47              |
| 14:CN:24:CYS:CB  | 14:CN:29:ARG:HB3  | 2.45                     | 0.47              |
| 14:CN:36:PHE:HE1 | 14:CN:37:PHE:CZ   | 2.33                     | 0.47              |
| 15:CO:9:GLN:O    | 15:CO:12:ILE:HB   | 2.15                     | 0.47              |
| 16:CP:74:LEU:O   | 16:CP:75:ARG:C    | 2.54                     | 0.47              |
| 6:CF:99:ALA:HB3  | 18:CR:29:PHE:CZ   | 2.50                     | 0.47              |
| 20:CT:46:GLU:HG2 | 20:CT:48:LYS:HE2  | 1.96                     | 0.47              |
| 21:CU:24:ARG:HG2 | 21:CU:24:ARG:HH11 | 1.79                     | 0.47              |
| 55:D6:10:LEU:HA  | 55:D6:25:LYS:HA   | 1.97                     | 0.47              |
| 55:D6:40:CYS:HB2 | 55:D6:46:HIS:CB   | 2.44                     | 0.47              |
| 57:D8:14:VAL:CG2 | 57:D8:15:LYS:N    | 2.77                     | 0.47              |
| 27:DA:1155:A:H4' | 43:DU:55:ARG:NH1  | 2.30                     | 0.47              |
| 27:DA:1722:A:C2  | 27:DA:1740:G:H8   | 2.33                     | 0.47              |
| 27:DA:191:A:C2   | 27:DA:192:C:C2    | 3.02                     | 0.47              |
| 27:DA:1982:C:H2' | 27:DA:1983:C:C6   | 2.49                     | 0.47              |
| 27:DA:1991:U:O2' | 27:DA:1992:G:C5'  | 2.62                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:200:U:C5'   | 27:DA:200:U:C6    | 2.91                     | 0.47              |
| 27:DA:2136:C:H2'  | 27:DA:2137:C:C6   | 2.47                     | 0.47              |
| 27:DA:2481:G:O2'  | 27:DA:2482:G:P    | 2.73                     | 0.47              |
| 27:DA:2543:G:H2'  | 27:DA:2544:G:O4'  | 2.15                     | 0.47              |
| 27:DA:2610:C:H4'  | 27:DA:2611:U:OP2  | 2.14                     | 0.47              |
| 27:DA:2716:U:C2'  | 27:DA:2717:G:H5'  | 2.44                     | 0.47              |
| 27:DA:271(A):A:C8 | 27:DA:271(B):C:C6 | 2.99                     | 0.47              |
| 27:DA:2807:G:C2'  | 27:DA:2808:U:H5'' | 2.44                     | 0.47              |
| 27:DA:614:U:O2    | 27:DA:614:U:O4'   | 2.31                     | 0.47              |
| 27:DA:792:G:H3'   | 27:DA:792:G:OP1   | 2.14                     | 0.47              |
| 27:DA:845:G:H5''  | 27:DA:845:G:H8    | 1.79                     | 0.47              |
| 27:DA:968:G:C2    | 27:DA:969:U:C2    | 3.03                     | 0.47              |
| 27:DA:1791:A:O2'  | 30:DD:207:GLY:CA  | 2.63                     | 0.47              |
| 30:DD:43:ARG:CB   | 30:DD:54:ARG:HB3  | 2.45                     | 0.47              |
| 27:DA:2572:A:OP1  | 31:DE:143:ASN:HB3 | 2.14                     | 0.47              |
| 31:DE:88:GLY:O    | 31:DE:89:ASP:HB2  | 2.14                     | 0.47              |
| 33:DG:20:ILE:HA   | 33:DG:25:TYR:CD2  | 2.48                     | 0.47              |
| 35:DI:125:GLU:OE1 | 35:DI:125:GLU:HA  | 2.14                     | 0.47              |
| 37:DO:29:ASN:O    | 37:DO:30:ALA:C    | 2.53                     | 0.47              |
| 38:DP:95:VAL:HG22 | 38:DP:125:VAL:HB  | 1.96                     | 0.47              |
| 39:DQ:109:VAL:CG1 | 39:DQ:113:GLN:HB3 | 2.44                     | 0.47              |
| 40:DR:28:LEU:HD23 | 40:DR:34:ILE:HG12 | 1.97                     | 0.47              |
| 40:DR:43:GLU:C    | 40:DR:45:ARG:N    | 2.67                     | 0.47              |
| 41:DS:29:PHE:CD2  | 41:DS:30:ARG:N    | 2.83                     | 0.47              |
| 42:DT:65:LYS:HA   | 42:DT:65:LYS:NZ   | 2.30                     | 0.47              |
| 48:DZ:109:GLY:HA3 | 48:DZ:144:GLU:OE1 | 2.15                     | 0.47              |
| 1:AA:1225:A:H3'   | 13:AM:103:THR:OG1 | 2.15                     | 0.46              |
| 1:AA:1255:G:H5''  | 3:AC:26:LYS:HZ2   | 1.79                     | 0.46              |
| 1:AA:1326:C:O2'   | 1:AA:1327:C:H5'   | 2.15                     | 0.46              |
| 1:AA:1331:G:H4'   | 1:AA:1331:G:OP1   | 2.15                     | 0.46              |
| 1:AA:183:G:H2'    | 1:AA:184:G:H8     | 1.80                     | 0.46              |
| 1:AA:222:U:H2'    | 1:AA:223:U:C6     | 2.50                     | 0.46              |
| 1:AA:620:C:H2'    | 1:AA:621:A:O4'    | 2.14                     | 0.46              |
| 1:AA:673:G:C6     | 1:AA:734:G:C6     | 3.03                     | 0.46              |
| 1:AA:886:G:H2'    | 1:AA:887:G:O4'    | 2.15                     | 0.46              |
| 2:AB:189:ASP:OD1  | 2:AB:205:ASP:OD1  | 2.32                     | 0.46              |
| 2:AB:28:PHE:HD2   | 2:AB:194:PRO:HD3  | 1.78                     | 0.46              |
| 2:AB:52:GLU:O     | 2:AB:56:ARG:HG2   | 2.15                     | 0.46              |
| 4:AD:9:CYS:HB2    | 4:AD:22:LYS:NZ    | 2.29                     | 0.46              |
| 5:AE:144:THR:O    | 5:AE:145:LYS:C    | 2.53                     | 0.46              |
| 5:AE:144:THR:C    | 5:AE:146:ALA:N    | 2.66                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:73:ASN:O      | 5:AE:75:THR:N      | 2.42                     | 0.46              |
| 7:AG:69:VAL:HG12   | 7:AG:69:VAL:O      | 2.15                     | 0.46              |
| 8:AH:38:ILE:HD11   | 8:AH:118:VAL:HB    | 1.97                     | 0.46              |
| 8:AH:38:ILE:O      | 8:AH:42:GLU:HG2    | 2.15                     | 0.46              |
| 7:AG:153:HIS:HB3   | 11:AK:58:PRO:HG3   | 1.98                     | 0.46              |
| 13:AM:91:ARG:HH22  | 13:AM:103:THR:HG22 | 1.80                     | 0.46              |
| 13:AM:54:VAL:O     | 13:AM:58:GLU:N     | 2.30                     | 0.46              |
| 13:AM:68:GLY:HA2   | 13:AM:71:ARG:NH2   | 2.19                     | 0.46              |
| 15:AO:81:LEU:CG    | 15:AO:82:ILE:N     | 2.78                     | 0.46              |
| 1:AA:377:G:OP1     | 16:AP:3:LYS:HD3    | 2.15                     | 0.46              |
| 19:AS:5:LEU:C      | 19:AS:6:LYS:HE3    | 2.36                     | 0.46              |
| 20:AT:26:ASN:HB3   | 20:AT:71:THR:HG23  | 1.96                     | 0.46              |
| 51:B2:55:ARG:O     | 51:B2:56:GLN:C     | 2.53                     | 0.46              |
| 53:B4:40:ILE:HG23  | 53:B4:59:VAL:CG2   | 2.45                     | 0.46              |
| 53:B4:62:CYS:C     | 53:B4:64:LYS:H     | 2.18                     | 0.46              |
| 55:B6:16:CYS:SG    | 55:B6:16:CYS:O     | 2.74                     | 0.46              |
| 55:B6:32:ASN:O     | 55:B6:33:LYS:CB    | 2.63                     | 0.46              |
| 27:BA:1049:C:C4    | 27:BA:1111:A:C2    | 3.03                     | 0.46              |
| 27:BA:1006:C:C2    | 27:BA:1138:G:N2    | 2.83                     | 0.46              |
| 27:BA:1310:G:C2'   | 27:BA:1311:G:H5'   | 2.45                     | 0.46              |
| 27:BA:1479:G:C5    | 27:BA:1480:G:C8    | 3.03                     | 0.46              |
| 27:BA:1613:G:N1    | 27:BA:1617:C:C2    | 2.83                     | 0.46              |
| 27:BA:1632:A:H2'   | 27:BA:1633:G:C8    | 2.50                     | 0.46              |
| 27:BA:1657:C:H2'   | 27:BA:1658:C:C6    | 2.51                     | 0.46              |
| 27:BA:2162:G:O2'   | 27:BA:2163:C:H5'   | 2.15                     | 0.46              |
| 27:BA:2656:U:O2    | 27:BA:2656:U:H2'   | 2.14                     | 0.46              |
| 27:BA:283:A:H4'    | 27:BA:284:U:OP2    | 2.14                     | 0.46              |
| 27:BA:2808:U:C5'   | 27:BA:2891:G:O6    | 2.61                     | 0.46              |
| 27:BA:559:G:C2'    | 27:BA:560:C:H5'    | 2.45                     | 0.46              |
| 27:BA:930:U:H4'    | 27:BA:931:G:O5'    | 2.16                     | 0.46              |
| 27:BA:945:A:H5'    | 27:BA:946:G:OP2    | 2.15                     | 0.46              |
| 30:BD:13:ARG:NH1   | 30:BD:13:ARG:HG3   | 2.30                     | 0.46              |
| 32:BF:2:LYS:HG2    | 32:BF:25:PRO:HB2   | 1.97                     | 0.46              |
| 34:BH:109:PHE:HD1  | 34:BH:109:PHE:H    | 1.62                     | 0.46              |
| 35:BI:109:ILE:HG22 | 35:BI:111:PRO:CD   | 2.44                     | 0.46              |
| 36:BN:41:ASP:O     | 43:BU:64:ARG:NE    | 2.44                     | 0.46              |
| 38:BP:124:LYS:HG3  | 38:BP:143:GLY:HA3  | 1.97                     | 0.46              |
| 38:BP:17:LYS:C     | 38:BP:19:VAL:N     | 2.68                     | 0.46              |
| 39:BQ:56:ARG:O     | 39:BQ:57:HIS:O     | 2.33                     | 0.46              |
| 42:BT:36:GLU:HB3   | 42:BT:38:ASN:OD1   | 2.16                     | 0.46              |
| 43:BU:65:ILE:O     | 43:BU:68:ALA:N     | 2.44                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:BY:46:LYS:C    | 47:BY:47:LYS:CG   | 2.83                     | 0.46              |
| 47:BY:62:GLU:OE1  | 47:BY:62:GLU:CA   | 2.63                     | 0.46              |
| 48:BZ:174:VAL:HB  | 48:BZ:175:PRO:HD2 | 1.97                     | 0.46              |
| 1:CA:1256:A:O3'   | 1:CA:1257:U:H4'   | 2.15                     | 0.46              |
| 1:CA:1523:G:H2'   | 1:CA:1524:C:C6    | 2.50                     | 0.46              |
| 1:CA:66:G:O2'     | 1:CA:173:U:C5     | 2.53                     | 0.46              |
| 1:CA:189(A):C:H2' | 1:CA:189(B):C:H6  | 1.81                     | 0.46              |
| 1:CA:218:C:O2'    | 1:CA:219:C:O5'    | 2.33                     | 0.46              |
| 1:CA:258:G:H2'    | 1:CA:259:G:H8     | 1.79                     | 0.46              |
| 1:CA:42:G:H2'     | 1:CA:43:C:O4'     | 2.15                     | 0.46              |
| 1:CA:47:C:H4'     | 1:CA:48:C:O5'     | 2.15                     | 0.46              |
| 1:CA:68:G:N1      | 1:CA:102:G:N1     | 2.63                     | 0.46              |
| 1:CA:836:G:H2'    | 1:CA:837:G:H8     | 1.80                     | 0.46              |
| 1:CA:838:G:H22    | 1:CA:840:C:H5'    | 1.80                     | 0.46              |
| 1:CA:570:G:C6     | 1:CA:873:A:C6     | 3.02                     | 0.46              |
| 2:CB:168:THR:HA   | 2:CB:171:ALA:HB2  | 1.97                     | 0.46              |
| 2:CB:75:LYS:C     | 2:CB:77:ALA:H     | 2.16                     | 0.46              |
| 3:CC:50:ALA:HB1   | 3:CC:70:VAL:HG11  | 1.98                     | 0.46              |
| 4:CD:204:ILE:HG12 | 4:CD:204:ILE:H    | 1.47                     | 0.46              |
| 5:CE:91:LEU:HG    | 5:CE:120:THR:HG21 | 1.96                     | 0.46              |
| 6:CF:89:MET:SD    | 18:CR:76:LEU:CD2  | 2.96                     | 0.46              |
| 7:CG:139:GLU:O    | 7:CG:140:ASP:C    | 2.52                     | 0.46              |
| 9:CI:126:SER:O    | 9:CI:127:LYS:HB3  | 2.15                     | 0.46              |
| 16:CP:45:THR:C    | 16:CP:47:ASP:N    | 2.68                     | 0.46              |
| 17:CQ:76:LEU:O    | 17:CQ:76:LEU:CG   | 2.63                     | 0.46              |
| 20:CT:84:LEU:HD13 | 20:CT:88:VAL:HG23 | 1.96                     | 0.46              |
| 49:D0:11:ARG:O    | 49:D0:14:ARG:NH2  | 2.48                     | 0.46              |
| 49:D0:40:GLN:HE21 | 49:D0:43:THR:HA   | 1.77                     | 0.46              |
| 50:D1:11:ARG:CB   | 50:D1:12:PRO:HD2  | 2.28                     | 0.46              |
| 27:DA:2755:C:C4   | 58:D9:19:ARG:NH1  | 2.83                     | 0.46              |
| 27:DA:1151:G:O2'  | 43:DU:77:SER:O    | 2.32                     | 0.46              |
| 27:DA:1162:G:HO2' | 27:DA:1163:G:H5'  | 1.79                     | 0.46              |
| 27:DA:819:A:C4    | 27:DA:1189:A:C2   | 3.02                     | 0.46              |
| 27:DA:749:C:H4'   | 27:DA:1271:G:N3   | 2.30                     | 0.46              |
| 27:DA:1335:U:O2'  | 27:DA:1336:A:H5'  | 2.16                     | 0.46              |
| 27:DA:1312:U:C4   | 27:DA:1603:A:N6   | 2.83                     | 0.46              |
| 27:DA:1677:A:H8   | 27:DA:1677:A:O5'  | 1.99                     | 0.46              |
| 27:DA:1812:A:H2'  | 27:DA:1813:G:C8   | 2.51                     | 0.46              |
| 27:DA:1830:C:O2'  | 27:DA:1831:G:H5'  | 2.16                     | 0.46              |
| 27:DA:2016:U:H5'' | 27:DA:2058:A:OP1  | 2.15                     | 0.46              |
| 27:DA:2160:G:H2'  | 27:DA:2161:C:C5   | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2418:A:C2    | 27:DA:2419:U:C2    | 3.03                     | 0.46              |
| 27:DA:249:C:C2'    | 27:DA:249:C:O2     | 2.63                     | 0.46              |
| 27:DA:2543:G:C2    | 27:DA:2544:G:N3    | 2.83                     | 0.46              |
| 27:DA:2559:C:O2    | 27:DA:2559:C:H2'   | 2.14                     | 0.46              |
| 27:DA:2581:G:C8    | 27:DA:2582:G:O6    | 2.68                     | 0.46              |
| 27:DA:753:C:O2     | 27:DA:753:C:C2'    | 2.63                     | 0.46              |
| 27:DA:847:U:H2'    | 27:DA:848:G:C5'    | 2.42                     | 0.46              |
| 27:DA:887:A:H2'    | 27:DA:888:C:H5''   | 1.97                     | 0.46              |
| 27:DA:999:U:O2     | 27:DA:1000:A:C8    | 2.67                     | 0.46              |
| 28:DB:17:C:H2'     | 28:DB:18:G:C8      | 2.48                     | 0.46              |
| 32:DF:132:VAL:CG2  | 32:DF:133:ASN:H    | 2.12                     | 0.46              |
| 34:DH:89:ILE:HD11  | 34:DH:129:THR:HG22 | 1.97                     | 0.46              |
| 34:DH:12:PRO:HG3   | 34:DH:50:VAL:HG23  | 1.96                     | 0.46              |
| 34:DH:53:GLU:O     | 34:DH:65:HIS:HD2   | 1.98                     | 0.46              |
| 35:DI:120:ILE:HG22 | 35:DI:122:GLU:H    | 1.80                     | 0.46              |
| 36:DN:112:LEU:O    | 36:DN:112:LEU:HD12 | 2.14                     | 0.46              |
| 36:DN:133:GLN:HG2  | 36:DN:135:PRO:CD   | 2.31                     | 0.46              |
| 36:DN:38:HIS:HA    | 43:DU:67:ALA:CB    | 2.45                     | 0.46              |
| 36:DN:90:MET:O     | 36:DN:92:ALA:N     | 2.48                     | 0.46              |
| 27:DA:811:U:OP2    | 38:DP:25:SER:N     | 2.47                     | 0.46              |
| 39:DQ:49:ALA:O     | 39:DQ:53:ALA:HB2   | 2.14                     | 0.46              |
| 41:DS:99:LYS:O     | 41:DS:101:LEU:HD12 | 2.15                     | 0.46              |
| 27:DA:2334:G:O4'   | 41:DS:15:ARG:HG3   | 2.15                     | 0.46              |
| 42:DT:110:ILE:HG22 | 42:DT:111:ARG:N    | 2.30                     | 0.46              |
| 42:DT:125:ARG:O    | 42:DT:128:GLU:HG2  | 2.14                     | 0.46              |
| 44:DV:76:LYS:O     | 44:DV:77:ALA:O     | 2.33                     | 0.46              |
| 47:DY:28:LYS:HG3   | 47:DY:37:VAL:HB    | 1.96                     | 0.46              |
| 47:DY:97:ARG:O     | 47:DY:98:VAL:HB    | 2.16                     | 0.46              |
| 48:DZ:94:PRO:HB2   | 48:DZ:126:LYS:NZ   | 2.30                     | 0.46              |
| 48:DZ:144:GLU:OE1  | 48:DZ:145:ILE:HG23 | 2.15                     | 0.46              |
| 48:DZ:157:PRO:HB2  | 48:DZ:158:PRO:CD   | 2.46                     | 0.46              |
| 1:AA:920:U:C1'     | 1:AA:1080:A:C2     | 2.99                     | 0.46              |
| 1:AA:1192:C:N4     | 1:AA:1193:G:C4     | 2.83                     | 0.46              |
| 1:AA:1206:G:O6     | 1:AA:1207:G:C6     | 2.68                     | 0.46              |
| 1:AA:250:A:H2      | 1:AA:274:A:N6      | 2.12                     | 0.46              |
| 1:AA:265:G:C2      | 1:AA:267:C:O4'     | 2.68                     | 0.46              |
| 1:AA:295:C:H2'     | 1:AA:296:U:O4'     | 2.15                     | 0.46              |
| 1:AA:940:C:OP1     | 7:AG:102:ARG:HD3   | 2.16                     | 0.46              |
| 2:AB:109:SER:C     | 2:AB:111:ARG:H     | 2.18                     | 0.46              |
| 2:AB:164:VAL:HB    | 2:AB:186:ALA:HB2   | 1.97                     | 0.46              |
| 2:AB:229:VAL:CG1   | 2:AB:230:VAL:N     | 2.78                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:80:ILE:HG21   | 2:AB:208:ILE:HG23  | 1.97                     | 0.46              |
| 8:AH:14:ARG:C      | 8:AH:16:ALA:H      | 2.18                     | 0.46              |
| 11:AK:105:VAL:HG23 | 11:AK:105:VAL:O    | 2.15                     | 0.46              |
| 15:AO:77:ARG:HA    | 15:AO:80:ALA:HB3   | 1.97                     | 0.46              |
| 16:AP:6:LEU:CD1    | 16:AP:6:LEU:N      | 2.77                     | 0.46              |
| 18:AR:22:VAL:O     | 18:AR:24:ALA:N     | 2.48                     | 0.46              |
| 20:AT:53:LEU:HA    | 20:AT:56:MET:HB3   | 1.97                     | 0.46              |
| 50:B1:8:SER:HB3    | 50:B1:66:HIS:CD2   | 2.50                     | 0.46              |
| 54:B5:40:LYS:HB2   | 54:B5:41:PRO:HD2   | 1.97                     | 0.46              |
| 55:B6:18:ARG:HB2   | 55:B6:19:ARG:H     | 1.39                     | 0.46              |
| 55:B6:35:GLU:OE1   | 55:B6:36:LEU:N     | 2.48                     | 0.46              |
| 27:BA:83:G:N2      | 27:BA:102:G:O2'    | 2.47                     | 0.46              |
| 27:BA:1055:G:H2'   | 27:BA:1108:U:H5'   | 1.97                     | 0.46              |
| 27:BA:107:C:C4     | 27:BA:108:U:C5     | 3.03                     | 0.46              |
| 27:BA:839:U:H1'    | 27:BA:1191:G:H1'   | 1.96                     | 0.46              |
| 27:BA:1411:C:N4    | 27:BA:1412:A:H62   | 2.13                     | 0.46              |
| 27:BA:1479:G:H5'   | 27:BA:1558:A:H2    | 1.80                     | 0.46              |
| 27:BA:2001:A:C2    | 27:BA:2002:G:C4    | 3.03                     | 0.46              |
| 27:BA:2024:G:O2'   | 27:BA:2025:C:H5'   | 2.14                     | 0.46              |
| 27:BA:2118:U:H5    | 27:BA:2149:G:H5'   | 1.79                     | 0.46              |
| 27:BA:2548:G:O5'   | 27:BA:2548:G:H8    | 1.99                     | 0.46              |
| 27:BA:319:C:H2'    | 27:BA:320:A:O4'    | 2.15                     | 0.46              |
| 27:BA:478:A:C6     | 27:BA:480:A:C6     | 3.04                     | 0.46              |
| 27:BA:616:G:C6     | 27:BA:618:C:C4     | 3.04                     | 0.46              |
| 29:BC:141:LYS:O    | 29:BC:142:ALA:HB2  | 2.14                     | 0.46              |
| 29:BC:212:VAL:O    | 29:BC:213:TYR:CB   | 2.63                     | 0.46              |
| 30:BD:13:ARG:HH11  | 30:BD:13:ARG:HG3   | 1.80                     | 0.46              |
| 30:BD:26:LYS:O     | 30:BD:27:THR:HB    | 2.15                     | 0.46              |
| 31:BE:134:ILE:H    | 31:BE:134:ILE:HD13 | 1.80                     | 0.46              |
| 31:BE:89:ASP:O     | 31:BE:90:THR:HB    | 2.16                     | 0.46              |
| 32:BF:154:VAL:HG22 | 32:BF:191:ARG:CB   | 2.45                     | 0.46              |
| 33:BG:97:ASP:O     | 33:BG:101:ILE:HG23 | 2.15                     | 0.46              |
| 37:BO:108:GLU:C    | 37:BO:110:GLY:N    | 2.64                     | 0.46              |
| 38:BP:91:PHE:CD2   | 38:BP:95:VAL:HG12  | 2.50                     | 0.46              |
| 41:BS:96:GLY:C     | 41:BS:98:VAL:N     | 2.68                     | 0.46              |
| 46:BX:17:ALA:O     | 46:BX:20:GLY:N     | 2.47                     | 0.46              |
| 46:BX:63:LYS:HG3   | 46:BX:63:LYS:O     | 2.15                     | 0.46              |
| 47:BY:27:VAL:HG12  | 47:BY:29:GLU:OE1   | 2.15                     | 0.46              |
| 1:CA:1207:G:H2'    | 1:CA:1208:C:H6     | 1.81                     | 0.46              |
| 1:CA:1401:G:O5'    | 1:CA:1401:G:H8     | 1.97                     | 0.46              |
| 1:CA:1405:G:O2'    | 1:CA:1406:U:H5'    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:152:A:N6     | 1:CA:170:U:C2     | 2.84                     | 0.46              |
| 1:CA:163:C:H2'    | 1:CA:164:U:C6     | 2.50                     | 0.46              |
| 1:CA:16:A:N1      | 1:CA:919:A:C2     | 2.75                     | 0.46              |
| 1:CA:624:C:O2'    | 1:CA:625:G:C5'    | 2.62                     | 0.46              |
| 1:CA:810:C:H2'    | 1:CA:811:C:H5'    | 1.96                     | 0.46              |
| 1:CA:823:G:O2'    | 1:CA:824:C:H5'    | 2.15                     | 0.46              |
| 1:CA:1075:C:P     | 2:CB:103:THR:HG21 | 2.55                     | 0.46              |
| 2:CB:19:HIS:ND1   | 2:CB:20:GLU:HG2   | 2.28                     | 0.46              |
| 2:CB:208:ILE:HA   | 2:CB:211:ILE:HB   | 1.97                     | 0.46              |
| 2:CB:97:TRP:HE3   | 2:CB:97:TRP:O     | 1.98                     | 0.46              |
| 3:CC:148:GLY:HA3  | 3:CC:203:PHE:HB3  | 1.97                     | 0.46              |
| 4:CD:57:ARG:NH2   | 5:CE:107:ARG:CZ   | 2.78                     | 0.46              |
| 8:CH:69:ARG:HH11  | 8:CH:77:GLU:N     | 2.13                     | 0.46              |
| 9:CI:125:TYR:HD2  | 9:CI:126:SER:N    | 2.12                     | 0.46              |
| 13:CM:112:GLY:HA2 | 13:CM:113:PRO:HD2 | 1.73                     | 0.46              |
| 1:CA:974:A:OP2    | 14:CN:41:ARG:NH1  | 2.48                     | 0.46              |
| 1:CA:1115:C:H1'   | 14:CN:61:TRP:O    | 2.15                     | 0.46              |
| 16:CP:82:GLN:O    | 16:CP:83:GLU:HB2  | 2.16                     | 0.46              |
| 22:CV:4:A:C2      | 22:CV:5:U:O2      | 2.68                     | 0.46              |
| 53:D4:37:PRO:O    | 53:D4:55:PRO:HG3  | 2.15                     | 0.46              |
| 54:D5:40:LYS:HB2  | 54:D5:41:PRO:HD2  | 1.96                     | 0.46              |
| 27:DA:1210:A:H5'  | 27:DA:1211:U:H3'  | 1.96                     | 0.46              |
| 27:DA:1385:G:O2'  | 27:DA:1396:U:C6   | 2.67                     | 0.46              |
| 27:DA:1669:A:H2'  | 27:DA:1670:C:H5'  | 1.96                     | 0.46              |
| 27:DA:1722:A:C6   | 27:DA:1741:A:C6   | 3.03                     | 0.46              |
| 27:DA:1952:A:C6   | 27:DA:1953:A:N1   | 2.83                     | 0.46              |
| 27:DA:1998:G:H4'  | 27:DA:2724:C:O2'  | 2.15                     | 0.46              |
| 27:DA:2093:G:C6   | 27:DA:2225:A:C8   | 3.03                     | 0.46              |
| 27:DA:2230:G:C6   | 27:DA:2231:C:C4   | 3.03                     | 0.46              |
| 27:DA:2276:G:N2   | 27:DA:2277:G:C5   | 2.83                     | 0.46              |
| 27:DA:2295:C:O2   | 27:DA:2338:G:C2   | 2.68                     | 0.46              |
| 27:DA:2406:U:C2   | 38:DP:72:PRO:HB2  | 2.49                     | 0.46              |
| 27:DA:2428:G:N2   | 38:DP:60:MET:HE1  | 2.30                     | 0.46              |
| 27:DA:2458:G:H8   | 27:DA:2458:G:O5'  | 1.98                     | 0.46              |
| 27:DA:2571:C:C3'  | 27:DA:2572:A:C5'  | 2.93                     | 0.46              |
| 27:DA:307:G:H22   | 27:DA:309:G:H3'   | 1.77                     | 0.46              |
| 27:DA:314:A:H2'   | 27:DA:315:G:C8    | 2.51                     | 0.46              |
| 27:DA:418:G:H2'   | 27:DA:419:C:H6    | 1.81                     | 0.46              |
| 27:DA:475:U:C2'   | 27:DA:476:G:C8    | 2.98                     | 0.46              |
| 27:DA:532:A:H4'   | 27:DA:533:G:C8    | 2.51                     | 0.46              |
| 27:DA:714:U:C2'   | 27:DA:715:G:H5''  | 2.43                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:888:C:H3'    | 27:DA:889:C:H5'    | 1.96                     | 0.46              |
| 27:DA:971:C:OP1    | 27:DA:974:G:C8     | 2.69                     | 0.46              |
| 27:DA:975(A):G:H2' | 27:DA:976:C:H6     | 1.81                     | 0.46              |
| 27:DA:9:U:H6       | 27:DA:9:U:O5'      | 1.98                     | 0.46              |
| 29:DC:182:PRO:O    | 29:DC:183:GLU:CB   | 2.61                     | 0.46              |
| 30:DD:270:ILE:C    | 30:DD:271:ILE:HG12 | 2.35                     | 0.46              |
| 31:DE:89:ASP:O     | 31:DE:90:THR:CB    | 2.63                     | 0.46              |
| 27:DA:2303:G:H1'   | 33:DG:132:ASN:HD22 | 1.78                     | 0.46              |
| 35:DI:19:VAL:HG22  | 35:DI:20:ASP:N     | 2.30                     | 0.46              |
| 35:DI:64:GLU:HA    | 35:DI:64:GLU:OE1   | 2.14                     | 0.46              |
| 36:DN:134:ARG:H    | 36:DN:135:PRO:HD3  | 1.80                     | 0.46              |
| 39:DQ:35:VAL:HB    | 39:DQ:102:VAL:HG22 | 1.97                     | 0.46              |
| 40:DR:51:LEU:CA    | 40:DR:54:LEU:HB2   | 2.43                     | 0.46              |
| 41:DS:38:GLN:HB3   | 41:DS:47:THR:HG23  | 1.96                     | 0.46              |
| 42:DT:27:THR:HG23  | 42:DT:28:VAL:N     | 2.30                     | 0.46              |
| 48:DZ:157:PRO:CB   | 48:DZ:158:PRO:CD   | 2.93                     | 0.46              |
| 48:DZ:13:LYS:HB3   | 48:DZ:16:ALA:HB3   | 1.96                     | 0.46              |
| 48:DZ:73:VAL:HG12  | 48:DZ:75:LEU:HD22  | 1.98                     | 0.46              |
| 1:AA:29:G:H1       | 1:AA:554:C:H42     | 1.63                     | 0.46              |
| 2:AB:194:PRO:HA    | 2:AB:200:ILE:CD1   | 2.44                     | 0.46              |
| 2:AB:223:ILE:HA    | 2:AB:226:ARG:HB3   | 1.97                     | 0.46              |
| 3:AC:48:TYR:O      | 3:AC:50:ALA:N      | 2.48                     | 0.46              |
| 5:AE:28:PHE:CD1    | 5:AE:28:PHE:N      | 2.83                     | 0.46              |
| 5:AE:46:GLY:O      | 5:AE:54:ALA:HB1    | 2.16                     | 0.46              |
| 7:AG:38:LEU:O      | 7:AG:40:ALA:N      | 2.48                     | 0.46              |
| 8:AH:84:ARG:O      | 8:AH:135:CYS:HB2   | 2.16                     | 0.46              |
| 8:AH:65:TYR:CD1    | 8:AH:65:TYR:N      | 2.84                     | 0.46              |
| 8:AH:17:THR:CB     | 8:AH:78:GLN:OE1    | 2.54                     | 0.46              |
| 3:AC:23:TYR:HA     | 10:AJ:11:PHE:CE1   | 2.51                     | 0.46              |
| 1:AA:1152:A:H5''   | 10:AJ:13:HIS:CD2   | 2.50                     | 0.46              |
| 12:AL:30:ARG:HA    | 12:AL:30:ARG:HE    | 1.80                     | 0.46              |
| 13:AM:116:THR:HG22 | 13:AM:117:VAL:H    | 1.79                     | 0.46              |
| 14:AN:13:THR:HG23  | 14:AN:20:ALA:HB2   | 1.97                     | 0.46              |
| 14:AN:40:CYS:HG    | 14:AN:43:CYS:HG    | 1.58                     | 0.46              |
| 15:AO:85:LEU:HD23  | 15:AO:85:LEU:N     | 2.31                     | 0.46              |
| 19:AS:24:ALA:O     | 19:AS:25:LYS:CB    | 2.60                     | 0.46              |
| 23:AW:23:G:C8      | 23:AW:23:G:H5'     | 2.45                     | 0.46              |
| 25:AY:42:G:OP2     | 25:AY:42:G:H8      | 1.98                     | 0.46              |
| 25:AY:69:C:H2'     | 25:AY:70:C:O4'     | 2.16                     | 0.46              |
| 49:B0:41:ARG:N     | 49:B0:41:ARG:HD2   | 2.29                     | 0.46              |
| 27:BA:468:G:N7     | 56:B7:39:ARG:NH2   | 2.64                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:592:G:H2'    | 57:B8:4:MET:HE3    | 1.97                     | 0.46              |
| 27:BA:1022:G:O6    | 36:BN:66:LYS:HE3   | 2.16                     | 0.46              |
| 27:BA:1138:G:H2'   | 27:BA:1139:G:O4'   | 2.15                     | 0.46              |
| 27:BA:1523:U:O2'   | 27:BA:1524:G:H5'   | 2.15                     | 0.46              |
| 27:BA:1438:U:C4    | 27:BA:1552:G:N2    | 2.83                     | 0.46              |
| 27:BA:1705:G:H2'   | 27:BA:1706:U:O4'   | 2.15                     | 0.46              |
| 27:BA:2019:A:H2'   | 27:BA:2020:A:O5'   | 2.15                     | 0.46              |
| 27:BA:2033:A:C5    | 27:BA:2036:C:C4    | 3.03                     | 0.46              |
| 27:BA:250:G:C6     | 27:BA:251:A:C6     | 3.04                     | 0.46              |
| 27:BA:2533:A:H2'   | 27:BA:2534:A:C5'   | 2.43                     | 0.46              |
| 27:BA:2858:C:H2'   | 27:BA:2859:G:O4'   | 2.16                     | 0.46              |
| 27:BA:512:G:HO2'   | 27:BA:513:A:H8     | 1.63                     | 0.46              |
| 27:BA:614:U:H5''   | 27:BA:614(A):U:OP2 | 2.16                     | 0.46              |
| 27:BA:643:A:N7     | 55:B6:42:TRP:HH2   | 2.14                     | 0.46              |
| 27:BA:845:G:H8     | 27:BA:845:G:OP2    | 1.97                     | 0.46              |
| 28:BB:1:U:H5       | 28:BB:2:C:C4       | 2.34                     | 0.46              |
| 30:BD:16:MET:HG3   | 30:BD:206:LEU:O    | 2.16                     | 0.46              |
| 31:BE:125:GLY:HA3  | 31:BE:134:ILE:O    | 2.15                     | 0.46              |
| 33:BG:9:ARG:C      | 33:BG:11:TYR:N     | 2.67                     | 0.46              |
| 35:BI:49:ALA:O     | 35:BI:53:ALA:N     | 2.46                     | 0.46              |
| 27:BA:1138:G:N3    | 36:BN:106:MET:HE1  | 2.31                     | 0.46              |
| 32:BF:34:TRP:HB2   | 38:BP:10:PRO:HB3   | 1.98                     | 0.46              |
| 38:BP:114:ILE:HD12 | 38:BP:115:LEU:H    | 1.81                     | 0.46              |
| 39:BQ:58:PHE:O     | 39:BQ:59:ARG:O     | 2.34                     | 0.46              |
| 39:BQ:75:THR:CB    | 39:BQ:87:LYS:HZ2   | 2.27                     | 0.46              |
| 41:BS:85:VAL:HB    | 41:BS:86:ALA:H     | 1.44                     | 0.46              |
| 42:BT:28:VAL:HG13  | 42:BT:45:PHE:O     | 2.14                     | 0.46              |
| 43:BU:27:LEU:N     | 43:BU:27:LEU:CD2   | 2.69                     | 0.46              |
| 45:BW:14:PRO:O     | 45:BW:16:LYS:N     | 2.48                     | 0.46              |
| 47:BY:2:ARG:C      | 47:BY:4:LYS:N      | 2.68                     | 0.46              |
| 48:BZ:107:PRO:C    | 48:BZ:109:GLY:N    | 2.67                     | 0.46              |
| 1:CA:1104:G:H2'    | 1:CA:1105:A:O4'    | 2.15                     | 0.46              |
| 1:CA:391:G:C6      | 1:CA:392:G:C5      | 3.04                     | 0.46              |
| 1:CA:522:C:O4'     | 1:CA:536:C:H4'     | 2.15                     | 0.46              |
| 1:CA:71:C:H2'      | 1:CA:72:C:H6       | 1.80                     | 0.46              |
| 1:CA:738:C:H2'     | 1:CA:739:C:C6      | 2.50                     | 0.46              |
| 1:CA:977:A:H8      | 1:CA:982:U:O4      | 1.99                     | 0.46              |
| 2:CB:21:ARG:O      | 2:CB:22:LYS:HB2    | 2.15                     | 0.46              |
| 7:CG:2:ALA:HB1     | 7:CG:5:ARG:O       | 2.14                     | 0.46              |
| 8:CH:24:THR:HG22   | 8:CH:25:ASP:N      | 2.22                     | 0.46              |
| 10:CJ:4:ILE:HD11   | 10:CJ:77:PRO:HA    | 1.96                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:CL:94:ARG:C     | 12:CL:95:TYR:CD1   | 2.89                     | 0.46              |
| 1:CA:1216:G:H5'    | 14:CN:5:ALA:HB2    | 1.98                     | 0.46              |
| 18:CR:74:ARG:HG3   | 18:CR:79:LEU:HD12  | 1.95                     | 0.46              |
| 20:CT:33:ILE:CD1   | 20:CT:62:LEU:HB3   | 2.43                     | 0.46              |
| 21:CU:12:LYS:HD2   | 21:CU:17:THR:HG1   | 1.81                     | 0.46              |
| 50:D1:69:LYS:O     | 50:D1:72:GLU:HB3   | 2.15                     | 0.46              |
| 52:D3:11:SER:OG    | 52:D3:12:PRO:HD2   | 2.15                     | 0.46              |
| 52:D3:5:LYS:HE2    | 52:D3:57:GLU:HB3   | 1.96                     | 0.46              |
| 27:DA:977:G:H1'    | 27:DA:1000:A:H61   | 1.81                     | 0.46              |
| 27:DA:1030:G:H21   | 58:D9:5:ALA:HB1    | 1.80                     | 0.46              |
| 27:DA:1048:A:C2    | 27:DA:1109:C:N4    | 2.81                     | 0.46              |
| 27:DA:1242:A:C2    | 38:DP:8:PRO:HG3    | 2.50                     | 0.46              |
| 27:DA:1311:G:O2'   | 27:DA:1312:U:C5    | 2.68                     | 0.46              |
| 27:DA:1628:G:O2'   | 27:DA:1629:U:H5'   | 2.15                     | 0.46              |
| 27:DA:1790:C:H2'   | 27:DA:1791:A:C5    | 2.50                     | 0.46              |
| 27:DA:1855:G:C2    | 27:DA:1856:G:C8    | 3.02                     | 0.46              |
| 27:DA:245:G:O6     | 57:D8:8:LYS:NZ     | 2.40                     | 0.46              |
| 27:DA:2553:G:C6    | 27:DA:2583:G:O2'   | 2.69                     | 0.46              |
| 27:DA:2618:G:O2'   | 27:DA:2619:C:H5'   | 2.16                     | 0.46              |
| 27:DA:2751:G:H2'   | 27:DA:2751:G:N3    | 2.30                     | 0.46              |
| 27:DA:319:C:C4     | 27:DA:320:A:N7     | 2.84                     | 0.46              |
| 27:DA:374:A:H3'    | 27:DA:375:C:C6     | 2.51                     | 0.46              |
| 27:DA:562:U:O2'    | 27:DA:572:A:O4'    | 2.33                     | 0.46              |
| 27:DA:80:G:O2'     | 27:DA:81:G:H5'     | 2.15                     | 0.46              |
| 27:DA:96:G:N2      | 27:DA:97:C:C2      | 2.83                     | 0.46              |
| 27:DA:998:C:H42    | 27:DA:1158:C:N4    | 2.14                     | 0.46              |
| 28:DB:11:C:H3'     | 28:DB:12:C:H6      | 1.80                     | 0.46              |
| 32:DF:61:GLY:O     | 32:DF:62:ARG:C     | 2.53                     | 0.46              |
| 33:DG:123:ASN:O    | 33:DG:126:ASP:CG   | 2.54                     | 0.46              |
| 33:DG:126:ASP:O    | 33:DG:128:ARG:N    | 2.41                     | 0.46              |
| 34:DH:132:ARG:HG2  | 34:DH:132:ARG:HH11 | 1.81                     | 0.46              |
| 36:DN:120:LEU:HD13 | 36:DN:122:VAL:HG23 | 1.96                     | 0.46              |
| 36:DN:79:PRO:C     | 36:DN:81:GLY:H     | 2.17                     | 0.46              |
| 37:DO:17:ARG:H     | 37:DO:46:ALA:HA    | 1.80                     | 0.46              |
| 38:DP:86:LYS:N     | 38:DP:117:GLU:O    | 2.48                     | 0.46              |
| 39:DQ:11:LYS:NZ    | 39:DQ:88:GLY:O     | 2.46                     | 0.46              |
| 40:DR:28:LEU:HD23  | 40:DR:34:ILE:CG1   | 2.46                     | 0.46              |
| 40:DR:51:LEU:HA    | 40:DR:54:LEU:HD22  | 1.98                     | 0.46              |
| 41:DS:21:THR:C     | 41:DS:23:ARG:N     | 2.68                     | 0.46              |
| 44:DV:38:LEU:HD13  | 44:DV:55:ALA:CB    | 2.43                     | 0.46              |
| 44:DV:72:VAL:HG23  | 44:DV:85:LYS:HB3   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:DY:76:CYS:CB   | 47:DY:77:PRO:HD2   | 2.45                     | 0.46              |
| 48:DZ:96:GLU:CB   | 48:DZ:124:LEU:HD11 | 2.42                     | 0.46              |
| 1:AA:99:U:H2'     | 1:AA:100:C:C6      | 2.49                     | 0.46              |
| 1:AA:1087:G:H2'   | 1:AA:1088:G:H8     | 1.79                     | 0.46              |
| 1:AA:1446:U:O2'   | 1:AA:1447:A:C8     | 2.66                     | 0.46              |
| 1:AA:268:C:C5     | 1:AA:269:C:C5      | 3.04                     | 0.46              |
| 1:AA:289:G:N2     | 1:AA:290:C:C2      | 2.83                     | 0.46              |
| 1:AA:44:G:H2'     | 1:AA:45:U:O4'      | 2.15                     | 0.46              |
| 1:AA:473:G:C4     | 1:AA:474:G:N7      | 2.84                     | 0.46              |
| 1:AA:481:G:H1'    | 1:AA:483:C:N4      | 2.29                     | 0.46              |
| 1:AA:828:A:H62    | 1:AA:858:G:H21     | 1.64                     | 0.46              |
| 1:AA:967:C:H2'    | 1:AA:968:A:N7      | 2.30                     | 0.46              |
| 2:AB:106:LYS:HG2  | 2:AB:107:THR:N     | 2.31                     | 0.46              |
| 2:AB:114:ARG:HD3  | 2:AB:117:GLU:OE1   | 2.16                     | 0.46              |
| 2:AB:69:LEU:HD22  | 2:AB:159:PRO:HG2   | 1.96                     | 0.46              |
| 2:AB:75:LYS:HD3   | 2:AB:78:GLN:CB     | 2.46                     | 0.46              |
| 3:AC:179:ARG:HD2  | 3:AC:207:VAL:HA    | 1.97                     | 0.46              |
| 4:AD:38:TYR:HB2   | 4:AD:44:GLY:O      | 2.16                     | 0.46              |
| 5:AE:72:GLN:NE2   | 5:AE:144:THR:CG2   | 2.78                     | 0.46              |
| 6:AF:33:TYR:CB    | 6:AF:75:LEU:HD12   | 2.41                     | 0.46              |
| 7:AG:38:LEU:C     | 7:AG:40:ALA:H      | 2.18                     | 0.46              |
| 11:AK:38:ASN:ND2  | 11:AK:38:ASN:H     | 2.12                     | 0.46              |
| 50:B1:4:VAL:HG22  | 50:B1:4:VAL:O      | 2.15                     | 0.46              |
| 51:B2:3:LEU:HA    | 51:B2:6:VAL:HG23   | 1.97                     | 0.46              |
| 54:B5:17:ASP:O    | 54:B5:20:ARG:HB2   | 2.16                     | 0.46              |
| 27:BA:1178:C:C6   | 27:BA:1179:C:C5    | 3.04                     | 0.46              |
| 27:BA:1303:G:H2'  | 27:BA:1304:C:H6    | 1.81                     | 0.46              |
| 27:BA:2144:U:H4'  | 27:BA:2145:C:C5    | 2.49                     | 0.46              |
| 27:BA:2366:A:H3'  | 27:BA:2367:G:H8    | 1.81                     | 0.46              |
| 27:BA:2508:G:O2'  | 27:BA:2509:G:H5'   | 2.14                     | 0.46              |
| 27:BA:2628:C:H4'  | 27:BA:2781:A:C5    | 2.51                     | 0.46              |
| 27:BA:574:C:H1'   | 27:BA:2055:C:C6    | 2.51                     | 0.46              |
| 27:BA:836:G:C5    | 27:BA:837:C:C4     | 3.04                     | 0.46              |
| 27:BA:906:G:H5'   | 39:BQ:26:TYR:HH    | 1.76                     | 0.46              |
| 27:BA:906:G:O3'   | 39:BQ:67:ARG:NH2   | 2.49                     | 0.46              |
| 28:BB:79:C:O2'    | 28:BB:80:U:H5'     | 2.15                     | 0.46              |
| 28:BB:91:C:H2'    | 28:BB:92:C:O5'     | 2.15                     | 0.46              |
| 32:BF:38:ARG:CG   | 32:BF:38:ARG:HH11  | 2.25                     | 0.46              |
| 34:BH:151:ILE:O   | 34:BH:152:ARG:HG2  | 2.15                     | 0.46              |
| 35:BI:92:VAL:HG12 | 35:BI:120:ILE:HB   | 1.97                     | 0.46              |
| 38:BP:146:VAL:CG2 | 38:BP:147:LEU:H    | 2.02                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 42:BT:29:ARG:HA    | 42:BT:29:ARG:HD3    | 1.49                     | 0.46              |
| 42:BT:28:VAL:CG1   | 42:BT:46:GLU:HA     | 2.45                     | 0.46              |
| 47:BY:10:GLY:HA2   | 47:BY:27:VAL:CG1    | 2.34                     | 0.46              |
| 1:CA:1128:C:H1'    | 1:CA:1146:A:H61     | 1.81                     | 0.46              |
| 1:CA:1261:A:H5'    | 1:CA:1283:G:O3'     | 2.16                     | 0.46              |
| 1:CA:23:C:C2'      | 1:CA:24:U:H5'       | 2.45                     | 0.46              |
| 1:CA:402:G:H4'     | 1:CA:620:C:O2       | 2.15                     | 0.46              |
| 1:CA:986:A:O2'     | 1:CA:987:G:H5'      | 2.15                     | 0.46              |
| 4:CD:202:LEU:HA    | 4:CD:205:GLU:OE2    | 2.16                     | 0.46              |
| 5:CE:129:ILE:HD12  | 5:CE:129:ILE:N      | 2.27                     | 0.46              |
| 10:CJ:39:PRO:HB3   | 10:CJ:70:ARG:HE     | 1.79                     | 0.46              |
| 10:CJ:80:LYS:HE3   | 10:CJ:80:LYS:C      | 2.36                     | 0.46              |
| 25:CY:67:C:H2'     | 25:CY:68:C:H6       | 1.81                     | 0.46              |
| 53:D4:48:ILE:HG22  | 53:D4:50:THR:HG23   | 1.96                     | 0.46              |
| 27:DA:2371:G:H4'   | 55:D6:45:LYS:HB2    | 1.95                     | 0.46              |
| 56:D7:13:ALA:O     | 56:D7:14:LYS:C      | 2.53                     | 0.46              |
| 58:D9:32:HIS:O     | 58:D9:34:GLN:HG3    | 2.15                     | 0.46              |
| 58:D9:22:ARG:CD    | 58:D9:35:ARG:HD2    | 2.46                     | 0.46              |
| 27:DA:1009:A:O2'   | 27:DA:1010:A:H5'    | 2.15                     | 0.46              |
| 27:DA:1021:A:C2    | 27:DA:1023:U:C2     | 3.02                     | 0.46              |
| 27:DA:1140:C:P     | 36:DN:66:LYS:HZ3    | 2.38                     | 0.46              |
| 27:DA:1142(A):A:C8 | 27:DA:1142(A):A:H5' | 2.43                     | 0.46              |
| 27:DA:1224:C:H6    | 27:DA:1224:C:OP1    | 1.97                     | 0.46              |
| 27:DA:1568:G:P     | 30:DD:61:LEU:HB2    | 2.55                     | 0.46              |
| 27:DA:1701:A:C3'   | 27:DA:1702:G:H5'    | 2.46                     | 0.46              |
| 27:DA:1772:G:N2    | 27:DA:1774:C:C5'    | 2.76                     | 0.46              |
| 27:DA:1956:U:C2'   | 27:DA:1957:C:H5'    | 2.45                     | 0.46              |
| 27:DA:2027:G:C5    | 27:DA:2028:U:C5     | 3.04                     | 0.46              |
| 27:DA:2673:G:O2'   | 27:DA:2674:G:H5'    | 2.16                     | 0.46              |
| 27:DA:302:C:H2'    | 27:DA:303:U:C6      | 2.50                     | 0.46              |
| 27:DA:363(B):G:H2' | 27:DA:363(C):G:C8   | 2.50                     | 0.46              |
| 27:DA:58:G:O2'     | 27:DA:59:U:H5'      | 2.14                     | 0.46              |
| 27:DA:691:C:H2'    | 27:DA:692:C:H6      | 1.79                     | 0.46              |
| 27:DA:93:G:C2'     | 27:DA:94:C:O4'      | 2.58                     | 0.46              |
| 27:DA:992:C:C3'    | 27:DA:992:C:C6      | 2.98                     | 0.46              |
| 30:DD:63:ARG:CD    | 30:DD:63:ARG:N      | 2.79                     | 0.46              |
| 31:DE:4:ILE:CD1    | 31:DE:31:CYS:SG     | 3.04                     | 0.46              |
| 27:DA:600:G:O3'    | 32:DF:108:LYS:HE3   | 2.15                     | 0.46              |
| 32:DF:109:GLY:HA2  | 32:DF:112:MET:HE3   | 1.98                     | 0.46              |
| 32:DF:124:LEU:HG   | 32:DF:126:VAL:CG1   | 2.45                     | 0.46              |
| 33:DG:15:VAL:HG13  | 33:DG:175:LEU:CD2   | 2.44                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DI:37:VAL:HG12 | 35:DI:38:LEU:CD1   | 2.34                     | 0.46              |
| 38:DP:114:ILE:O   | 38:DP:114:ILE:HG23 | 2.15                     | 0.46              |
| 38:DP:80:TYR:CD1  | 38:DP:111:ARG:HB3  | 2.50                     | 0.46              |
| 40:DR:6:SER:C     | 40:DR:7:GLY:O      | 2.54                     | 0.46              |
| 41:DS:97:ARG:NH2  | 41:DS:99:LYS:N     | 2.62                     | 0.46              |
| 43:DU:12:ARG:HA   | 43:DU:15:LYS:NZ    | 2.31                     | 0.46              |
| 47:DY:28:LYS:CA   | 47:DY:39:VAL:H     | 2.29                     | 0.46              |
| 48:DZ:79:ARG:O    | 48:DZ:81:ARG:N     | 2.49                     | 0.46              |
| 1:AA:292:G:C5     | 1:AA:293:G:H1'     | 2.51                     | 0.46              |
| 1:AA:658:G:C6     | 1:AA:749:C:N4      | 2.84                     | 0.46              |
| 1:AA:953:G:O6     | 1:AA:1228:C:N4     | 2.42                     | 0.46              |
| 2:AB:75:LYS:HE3   | 2:AB:78:GLN:NE2    | 2.31                     | 0.46              |
| 3:AC:154:SER:OG   | 3:AC:155:GLY:N     | 2.48                     | 0.46              |
| 3:AC:175:LEU:C    | 3:AC:177:THR:H     | 2.19                     | 0.46              |
| 8:AH:20:TYR:HD1   | 8:AH:65:TYR:HD2    | 1.63                     | 0.46              |
| 9:AI:53:VAL:CG2   | 9:AI:55:ALA:H      | 2.12                     | 0.46              |
| 10:AJ:21:GLN:O    | 10:AJ:21:GLN:HG2   | 2.15                     | 0.46              |
| 12:AL:22:PRO:O    | 12:AL:24:LEU:HD22  | 2.15                     | 0.46              |
| 12:AL:2:PRO:HA    | 12:AL:6:GLN:NE2    | 2.31                     | 0.46              |
| 13:AM:24:GLY:O    | 13:AM:25:ILE:HD12  | 2.15                     | 0.46              |
| 17:AQ:66:SER:O    | 17:AQ:67:LYS:C     | 2.52                     | 0.46              |
| 18:AR:22:VAL:O    | 18:AR:23:LYS:C     | 2.54                     | 0.46              |
| 50:B1:52:ARG:O    | 50:B1:56:GLN:O     | 2.33                     | 0.46              |
| 51:B2:5:GLU:O     | 51:B2:9:GLN:HB2    | 2.15                     | 0.46              |
| 27:BA:2350:C:H5'  | 57:B8:42:ARG:HD3   | 1.98                     | 0.46              |
| 27:BA:1042:G:H1   | 27:BA:1112:G:H22   | 1.63                     | 0.46              |
| 27:BA:1224:C:H6   | 27:BA:1224:C:OP1   | 1.98                     | 0.46              |
| 27:BA:489:G:C4    | 27:BA:1284:A:C6    | 3.04                     | 0.46              |
| 27:BA:1468:C:C4   | 27:BA:1525:G:C2    | 3.04                     | 0.46              |
| 27:BA:1802:A:C6   | 27:BA:1803:A:C6    | 3.03                     | 0.46              |
| 27:BA:196:A:OP2   | 38:BP:46:LYS:NZ    | 2.44                     | 0.46              |
| 27:BA:245:G:C2'   | 27:BA:246:C:H5'    | 2.45                     | 0.46              |
| 27:BA:374:A:C2    | 27:BA:401:A:C4     | 3.04                     | 0.46              |
| 27:BA:566:U:O4    | 44:BV:78:LYS:HE3   | 2.15                     | 0.46              |
| 27:BA:571:A:O2'   | 27:BA:573:G:O5'    | 2.23                     | 0.46              |
| 27:BA:826:U:H5'   | 27:BA:827:U:P      | 2.55                     | 0.46              |
| 29:BC:41:VAL:HG23 | 29:BC:178:ALA:CB   | 2.45                     | 0.46              |
| 30:BD:226:MET:HB3 | 30:BD:230:ASP:HB3  | 1.97                     | 0.46              |
| 31:BE:145:LYS:O   | 31:BE:148:GLY:CA   | 2.62                     | 0.46              |
| 27:BA:2729:G:C1'  | 31:BE:187:ALA:HB2  | 2.23                     | 0.46              |
| 32:BF:119:ARG:C   | 32:BF:121:GLY:N    | 2.67                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BG:149:VAL:O   | 33:BG:149:VAL:CG2  | 2.64                     | 0.46              |
| 33:BG:58:GLN:HG3  | 33:BG:59:GLU:N     | 2.30                     | 0.46              |
| 35:BI:131:LYS:CG  | 35:BI:132:PRO:CD   | 2.92                     | 0.46              |
| 36:BN:43:THR:HG22 | 36:BN:45:ASN:H     | 1.79                     | 0.46              |
| 36:BN:91:LEU:HD23 | 36:BN:98:VAL:HG21  | 1.97                     | 0.46              |
| 39:BQ:103:MET:HB2 | 39:BQ:104:PHE:CD1  | 2.50                     | 0.46              |
| 40:BR:79:LEU:HD23 | 40:BR:83:ILE:HB    | 1.95                     | 0.46              |
| 41:BS:20:ARG:HG2  | 41:BS:20:ARG:HH11  | 1.81                     | 0.46              |
| 43:BU:62:ILE:O    | 43:BU:65:ILE:N     | 2.48                     | 0.46              |
| 47:BY:27:VAL:O    | 47:BY:29:GLU:OE1   | 2.33                     | 0.46              |
| 47:BY:74:PRO:O    | 47:BY:75:ILE:HB    | 2.15                     | 0.46              |
| 1:CA:1046:A:H2'   | 1:CA:1047:G:O4'    | 2.16                     | 0.46              |
| 1:CA:1049:U:H2'   | 1:CA:1049:U:O2     | 2.15                     | 0.46              |
| 1:CA:1225:A:C5'   | 13:CM:103:THR:OG1  | 2.63                     | 0.46              |
| 1:CA:1273:G:H2'   | 1:CA:1274:G:C8     | 2.49                     | 0.46              |
| 1:CA:25:C:C2'     | 1:CA:26:A:H5'      | 2.45                     | 0.46              |
| 1:CA:260:G:H2'    | 1:CA:261:U:C6      | 2.50                     | 0.46              |
| 1:CA:725:G:H2'    | 1:CA:726:C:C6      | 2.50                     | 0.46              |
| 1:CA:935:A:HO2'   | 1:CA:936:C:P       | 2.39                     | 0.46              |
| 1:CA:995:C:O2'    | 1:CA:996:A:OP2     | 2.27                     | 0.46              |
| 2:CB:152:PHE:O    | 2:CB:154:LEU:N     | 2.48                     | 0.46              |
| 2:CB:228:GLY:O    | 2:CB:229:VAL:C     | 2.53                     | 0.46              |
| 2:CB:76:GLN:O     | 2:CB:77:ALA:CB     | 2.64                     | 0.46              |
| 2:CB:84:GLU:OE2   | 2:CB:216:SER:HA    | 2.15                     | 0.46              |
| 3:CC:134:ILE:HG22 | 3:CC:135:LYS:N     | 2.30                     | 0.46              |
| 5:CE:70:PRO:HB3   | 5:CE:144:THR:HG23  | 1.97                     | 0.46              |
| 49:D0:84:LEU:H    | 49:D0:84:LEU:HD12  | 1.81                     | 0.46              |
| 27:DA:1218:C:O2   | 27:DA:1218:C:H2'   | 2.15                     | 0.46              |
| 27:DA:1246:A:P    | 38:DP:16:ARG:NH2   | 2.89                     | 0.46              |
| 27:DA:1300:U:O2'  | 27:DA:1301:A:C5'   | 2.64                     | 0.46              |
| 27:DA:149:A:C2'   | 27:DA:150:C:O5'    | 2.63                     | 0.46              |
| 27:DA:1590:U:C2'  | 27:DA:1591:G:H5''  | 2.40                     | 0.46              |
| 27:DA:1349:A:N6   | 27:DA:1598:C:H42   | 2.12                     | 0.46              |
| 27:DA:1920:C:O2'  | 27:DA:1921:G:H5'   | 2.15                     | 0.46              |
| 27:DA:2247:A:C4   | 27:DA:2248:C:C5    | 3.04                     | 0.46              |
| 27:DA:2290:G:H2'  | 27:DA:2291:U:O4'   | 2.15                     | 0.46              |
| 27:DA:245:G:C6    | 27:DA:254:G:N2     | 2.83                     | 0.46              |
| 27:DA:2657:A:C2'  | 27:DA:2658:C:H5'   | 2.46                     | 0.46              |
| 27:DA:2712:U:H6   | 27:DA:2712(A):A:C8 | 2.34                     | 0.46              |
| 27:DA:675:A:OP1   | 32:DF:63:LYS:NZ    | 2.40                     | 0.46              |
| 27:DA:704:G:O2'   | 27:DA:705:A:O5'    | 2.30                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:727:A:O2'   | 27:DA:728:G:O4'    | 2.34                     | 0.46              |
| 27:DA:845:G:O2'   | 27:DA:846:C:C5     | 2.67                     | 0.46              |
| 27:DA:984:A:O5'   | 27:DA:984:A:H8     | 1.99                     | 0.46              |
| 27:DA:986:C:O2    | 27:DA:986:C:H2'    | 2.15                     | 0.46              |
| 28:DB:24:G:H4'    | 28:DB:25:A:C5'     | 2.44                     | 0.46              |
| 29:DC:194:ARG:O   | 29:DC:196:LEU:N    | 2.48                     | 0.46              |
| 29:DC:37:PHE:CD1  | 29:DC:39:GLU:HG3   | 2.51                     | 0.46              |
| 30:DD:154:LYS:HB2 | 30:DD:155:LEU:HD13 | 1.97                     | 0.46              |
| 31:DE:117:MET:O   | 31:DE:118:LYS:CB   | 2.59                     | 0.46              |
| 31:DE:55:ASN:HA   | 31:DE:55:ASN:HD22  | 1.50                     | 0.46              |
| 31:DE:59:VAL:HG21 | 31:DE:63:LEU:CG    | 2.44                     | 0.46              |
| 31:DE:59:VAL:HG13 | 31:DE:60:ASN:H     | 1.78                     | 0.46              |
| 31:DE:61:ARG:HB3  | 31:DE:62:PRO:CD    | 2.45                     | 0.46              |
| 27:DA:608:A:OP1   | 32:DF:100:THR:HG21 | 2.15                     | 0.46              |
| 33:DG:101:ILE:C   | 33:DG:101:ILE:HD13 | 2.36                     | 0.46              |
| 35:DI:66:GLU:C    | 35:DI:68:LEU:H     | 2.18                     | 0.46              |
| 37:DO:104:ARG:CZ  | 37:DO:104:ARG:HB3  | 2.45                     | 0.46              |
| 37:DO:87:ILE:HG23 | 37:DO:92:GLU:N     | 2.30                     | 0.46              |
| 39:DQ:37:LEU:HB2  | 39:DQ:128:LYS:O    | 2.16                     | 0.46              |
| 40:DR:11:ASN:O    | 40:DR:12:ARG:CB    | 2.63                     | 0.46              |
| 40:DR:69:ASP:OD2  | 40:DR:69:ASP:N     | 2.49                     | 0.46              |
| 41:DS:10:ARG:O    | 41:DS:11:LYS:C     | 2.54                     | 0.46              |
| 42:DT:124:ASP:C   | 42:DT:126:ALA:H    | 2.19                     | 0.46              |
| 42:DT:62:THR:CA   | 42:DT:74:ARG:O     | 2.62                     | 0.46              |
| 46:DX:36:LYS:HG2  | 46:DX:56:THR:CG2   | 2.45                     | 0.46              |
| 27:DA:84:A:P      | 47:DY:9:LYS:NZ     | 2.89                     | 0.46              |
| 1:AA:1392:G:N2    | 1:AA:1502:A:C8     | 2.83                     | 0.46              |
| 1:AA:1514:C:C4    | 1:AA:1515:C:C5     | 3.03                     | 0.46              |
| 1:AA:66:G:H5'     | 1:AA:173:U:O4      | 2.16                     | 0.46              |
| 1:AA:457:C:N3     | 1:AA:475:G:C2      | 2.83                     | 0.46              |
| 2:AB:229:VAL:HG12 | 2:AB:230:VAL:N     | 2.31                     | 0.46              |
| 3:AC:59:ARG:O     | 10:AJ:93:GLY:HA2   | 2.16                     | 0.46              |
| 4:AD:173:TRP:CE2  | 4:AD:189:PRO:HB3   | 2.50                     | 0.46              |
| 5:AE:80:ILE:CD1   | 5:AE:142:LEU:HD21  | 2.46                     | 0.46              |
| 7:AG:116:ALA:O    | 7:AG:120:ILE:HG12  | 2.15                     | 0.46              |
| 7:AG:143:ARG:O    | 7:AG:145:ALA:O     | 2.33                     | 0.46              |
| 8:AH:65:TYR:HD1   | 8:AH:65:TYR:N      | 2.13                     | 0.46              |
| 9:AI:111:ARG:HD2  | 14:AN:61:TRP:NE1   | 2.30                     | 0.46              |
| 10:AJ:95:GLU:CD   | 10:AJ:96:ILE:N     | 2.67                     | 0.46              |
| 12:AL:42:PRO:HB3  | 12:AL:89:ASP:HB3   | 1.98                     | 0.46              |
| 12:AL:84:GLY:HA2  | 12:AL:95:TYR:HA    | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:84:ILE:HG22  | 19:AS:74:PHE:HD1   | 1.81                     | 0.46              |
| 14:AN:32:SER:OG    | 14:AN:41:ARG:HG2   | 2.15                     | 0.46              |
| 24:AX:25:C:C2      | 24:AX:26:G:C8      | 3.03                     | 0.46              |
| 25:AY:47:C:C2      | 25:AY:58:A:H1'     | 2.51                     | 0.46              |
| 49:B0:14:ARG:O     | 49:B0:15:ASP:HB2   | 2.14                     | 0.46              |
| 55:B6:26:ASN:CB    | 55:B6:32:ASN:OD1   | 2.63                     | 0.46              |
| 57:B8:23:VAL:HG13  | 57:B8:47:LYS:O     | 2.16                     | 0.46              |
| 27:BA:1230:C:H2'   | 27:BA:1231:G:C8    | 2.51                     | 0.46              |
| 27:BA:2005:A:H2'   | 27:BA:2006:C:H5'   | 1.98                     | 0.46              |
| 27:BA:2171:A:HO2'  | 27:BA:2172:U:P     | 2.38                     | 0.46              |
| 27:BA:2726:U:O4'   | 27:BA:2726:U:O2    | 2.30                     | 0.46              |
| 27:BA:2741:A:H2'   | 27:BA:2742:C:O4'   | 2.15                     | 0.46              |
| 27:BA:363(A):A:H5' | 27:BA:363(B):G:P   | 2.56                     | 0.46              |
| 27:BA:489:G:C6     | 27:BA:491:G:C6     | 3.04                     | 0.46              |
| 27:BA:517:C:C2'    | 27:BA:518:G:H5'    | 2.45                     | 0.46              |
| 27:BA:628:G:H2'    | 27:BA:629:G:H8     | 1.80                     | 0.46              |
| 27:BA:753:C:C2'    | 27:BA:754:C:C5'    | 2.93                     | 0.46              |
| 27:BA:784:A:C5     | 30:BD:229:VAL:HG21 | 2.50                     | 0.46              |
| 27:BA:819:A:H2'    | 27:BA:820:A:O5'    | 2.16                     | 0.46              |
| 27:BA:844:C:H2'    | 27:BA:845:G:C8     | 2.50                     | 0.46              |
| 27:BA:92:A:O2'     | 27:BA:93:G:P       | 2.73                     | 0.46              |
| 30:BD:4:LYS:HD2    | 30:BD:18:VAL:CG2   | 2.46                     | 0.46              |
| 30:BD:31:LYS:O     | 30:BD:35:LYS:HB2   | 2.15                     | 0.46              |
| 30:BD:45:ASN:CG    | 30:BD:46:GLN:N     | 2.68                     | 0.46              |
| 31:BE:45:THR:O     | 31:BE:46:ALA:CB    | 2.64                     | 0.46              |
| 31:BE:47:VAL:O     | 31:BE:80:GLU:HA    | 2.16                     | 0.46              |
| 37:BO:17:ARG:NE    | 37:BO:47:ILE:HD13  | 2.28                     | 0.46              |
| 40:BR:30:THR:OG1   | 40:BR:75:LEU:HD21  | 2.14                     | 0.46              |
| 43:BU:96:ALA:O     | 43:BU:98:LEU:N     | 2.49                     | 0.46              |
| 47:BY:87:LYS:NZ    | 47:BY:89:PHE:CE1   | 2.83                     | 0.46              |
| 47:BY:88:LYS:HB3   | 47:BY:90:LEU:CD1   | 2.46                     | 0.46              |
| 48:BZ:111:ARG:NH1  | 48:BZ:111:ARG:HG2  | 2.25                     | 0.46              |
| 1:CA:1057:G:C5     | 1:CA:1204:A:C2     | 3.03                     | 0.46              |
| 1:CA:147:G:H1      | 1:CA:175:C:N4      | 2.12                     | 0.46              |
| 1:CA:250:A:H2      | 1:CA:274:A:N6      | 2.10                     | 0.46              |
| 1:CA:251:G:H4'     | 1:CA:252:U:O5'     | 2.16                     | 0.46              |
| 1:CA:264:U:C4      | 1:CA:265:G:C5      | 3.04                     | 0.46              |
| 1:CA:274:A:O2'     | 1:CA:275:G:P       | 2.74                     | 0.46              |
| 1:CA:399:G:C6      | 1:CA:400:C:C4      | 3.03                     | 0.46              |
| 1:CA:46:G:H2'      | 1:CA:366:C:C5      | 2.51                     | 0.46              |
| 1:CA:542:G:H5'     | 4:CD:41:GLY:HA3    | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:658:G:O2'     | 1:CA:659:U:H5'     | 2.15                     | 0.46              |
| 1:CA:668:G:H2'     | 1:CA:669:U:H6      | 1.81                     | 0.46              |
| 1:CA:715:A:H2'     | 1:CA:716:A:C8      | 2.51                     | 0.46              |
| 1:CA:775:G:O2'     | 1:CA:776:G:H5'     | 2.15                     | 0.46              |
| 1:CA:949:A:H1'     | 1:CA:1364:U:H3     | 1.80                     | 0.46              |
| 3:CC:114:PRO:HA    | 3:CC:185:GLY:HA3   | 1.98                     | 0.46              |
| 6:CF:42:GLU:C      | 6:CF:44:GLY:N      | 2.68                     | 0.46              |
| 8:CH:109:ILE:CG1   | 8:CH:120:THR:HB    | 2.46                     | 0.46              |
| 1:CA:876:G:P       | 8:CH:14:ARG:HH11   | 2.38                     | 0.46              |
| 8:CH:68:ARG:NH1    | 8:CH:68:ARG:CG     | 2.78                     | 0.46              |
| 20:CT:50:GLU:HA    | 20:CT:100:ILE:CG1  | 2.30                     | 0.46              |
| 20:CT:75:ASN:O     | 20:CT:76:ALA:C     | 2.54                     | 0.46              |
| 50:D1:56:GLN:OE1   | 50:D1:87:PRO:HD3   | 2.16                     | 0.46              |
| 52:D3:23:LEU:CA    | 52:D3:26:LEU:HD12  | 2.37                     | 0.46              |
| 52:D3:7:LYS:HB2    | 52:D3:34:GLU:HG2   | 1.98                     | 0.46              |
| 52:D3:8:LEU:HD22   | 52:D3:31:LEU:HD21  | 1.97                     | 0.46              |
| 57:D8:36:LYS:O     | 57:D8:37:SER:C     | 2.54                     | 0.46              |
| 27:DA:1205:U:H3'   | 27:DA:1206:G:H5'   | 1.98                     | 0.46              |
| 27:DA:1263:U:C4    | 27:DA:1264:G:C6    | 3.04                     | 0.46              |
| 27:DA:1349:A:N3    | 27:DA:1349:A:H5'   | 2.30                     | 0.46              |
| 27:DA:1599:C:H2'   | 27:DA:1600:C:C6    | 2.50                     | 0.46              |
| 27:DA:1628:G:H2'   | 27:DA:1629:U:C6    | 2.50                     | 0.46              |
| 27:DA:2282:G:H5''  | 27:DA:2283:C:O4'   | 2.16                     | 0.46              |
| 27:DA:2515:C:O2'   | 27:DA:2516:G:H5'   | 2.16                     | 0.46              |
| 27:DA:2572:A:O3'   | 27:DA:2574:G:H5''  | 2.16                     | 0.46              |
| 27:DA:2645:G:OP2   | 27:DA:2645:G:C8    | 2.69                     | 0.46              |
| 27:DA:271(Y):U:O2' | 27:DA:271(Z):C:OP2 | 2.34                     | 0.46              |
| 27:DA:284:U:O2'    | 27:DA:285:C:O4'    | 2.33                     | 0.46              |
| 27:DA:460:A:H3'    | 27:DA:461:C:H6     | 1.81                     | 0.46              |
| 27:DA:509:C:O2'    | 27:DA:510:C:C5'    | 2.64                     | 0.46              |
| 27:DA:565:C:H2'    | 27:DA:566:U:O4'    | 2.15                     | 0.46              |
| 27:DA:631:A:O2'    | 27:DA:632:A:H5'    | 2.15                     | 0.46              |
| 27:DA:675:A:C8     | 27:DA:804:A:C6     | 3.03                     | 0.46              |
| 27:DA:887:A:O2'    | 27:DA:888:C:H5''   | 2.16                     | 0.46              |
| 27:DA:906:G:C3'    | 27:DA:907:U:H5''   | 2.45                     | 0.46              |
| 27:DA:942:G:H1'    | 27:DA:1189:A:C2    | 2.51                     | 0.46              |
| 27:DA:957:A:H2     | 27:DA:2459:A:OP1   | 1.98                     | 0.46              |
| 27:DA:96:G:N1      | 27:DA:97:C:C4      | 2.84                     | 0.46              |
| 29:DC:56:GLN:HE22  | 29:DC:173:ALA:HB1  | 1.81                     | 0.46              |
| 31:DE:9:VAL:HG13   | 31:DE:10:GLY:H     | 1.80                     | 0.46              |
| 32:DF:179:GLU:H    | 32:DF:179:GLU:CD   | 2.19                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DG:97:ASP:O    | 33:DG:101:ILE:HG22 | 2.15                     | 0.46              |
| 34:DH:16:SER:HB3  | 34:DH:18:GLU:HG3   | 1.98                     | 0.46              |
| 37:DO:71:ARG:HH12 | 42:DT:74:ARG:NH2   | 2.07                     | 0.46              |
| 38:DP:16:ARG:O    | 38:DP:18:ARG:N     | 2.48                     | 0.46              |
| 41:DS:19:LYS:O    | 41:DS:19:LYS:HG2   | 2.15                     | 0.46              |
| 41:DS:61:ASN:O    | 41:DS:62:LYS:CG    | 2.63                     | 0.46              |
| 42:DT:28:VAL:HG11 | 42:DT:46:GLU:CG    | 2.46                     | 0.46              |
| 27:DA:560:C:H5''  | 43:DU:52:ARG:HH22  | 1.79                     | 0.46              |
| 45:DW:11:ARG:C    | 45:DW:11:ARG:NE    | 2.69                     | 0.46              |
| 45:DW:6:ILE:CG2   | 45:DW:8:ARG:HG3    | 2.45                     | 0.46              |
| 46:DX:31:HIS:CE1  | 46:DX:32:PRO:HG2   | 2.51                     | 0.46              |
| 47:DY:95:LYS:CD   | 47:DY:100:ALA:HA   | 2.45                     | 0.46              |
| 48:DZ:156:LEU:H   | 48:DZ:156:LEU:HD12 | 1.80                     | 0.46              |
| 1:AA:1301:U:H3'   | 1:AA:1302:U:H5''   | 1.98                     | 0.46              |
| 1:AA:184:G:O4'    | 1:AA:224:C:H4'     | 2.16                     | 0.46              |
| 1:AA:203:U:H1'    | 1:AA:216:G:N1      | 2.30                     | 0.46              |
| 1:AA:255:G:O3'    | 17:AQ:17:LYS:NZ    | 2.49                     | 0.46              |
| 1:AA:671:G:O2'    | 1:AA:672:U:H5'     | 2.15                     | 0.46              |
| 1:AA:756:C:H2'    | 1:AA:757:U:C6      | 2.51                     | 0.46              |
| 1:AA:9:G:OP2      | 5:AE:121:LYS:NZ    | 2.48                     | 0.46              |
| 2:AB:178:ARG:HH12 | 2:AB:196:LEU:HB3   | 1.77                     | 0.46              |
| 3:AC:64:VAL:O     | 3:AC:66:VAL:HG23   | 2.16                     | 0.46              |
| 5:AE:132:ALA:O    | 5:AE:135:THR:N     | 2.49                     | 0.46              |
| 6:AF:61:LEU:HB3   | 6:AF:62:TRP:H      | 1.53                     | 0.46              |
| 6:AF:9:VAL:O      | 6:AF:86:ARG:N      | 2.49                     | 0.46              |
| 13:AM:13:LYS:O    | 13:AM:44:ARG:HA    | 2.15                     | 0.46              |
| 13:AM:67:GLU:OE2  | 13:AM:68:GLY:N     | 2.49                     | 0.46              |
| 33:BG:2:PRO:HG2   | 53:B4:51:TYR:CG    | 2.49                     | 0.46              |
| 27:BA:2371:G:H4'  | 55:B6:45:LYS:HB2   | 1.98                     | 0.46              |
| 58:B9:13:LYS:HD3  | 58:B9:28:GLU:CG    | 2.40                     | 0.46              |
| 27:BA:1280:G:N3   | 27:BA:1280:G:H2'   | 2.30                     | 0.46              |
| 27:BA:1300:U:O2'  | 27:BA:1301:A:H5'   | 2.16                     | 0.46              |
| 27:BA:1365:A:N6   | 27:BA:1366:A:C6    | 2.84                     | 0.46              |
| 27:BA:1385:G:O2'  | 27:BA:1386:C:C6    | 2.68                     | 0.46              |
| 27:BA:158:U:O3'   | 27:BA:171:G:C8     | 2.62                     | 0.46              |
| 27:BA:1710:C:O2   | 27:BA:1749:A:C2    | 2.69                     | 0.46              |
| 27:BA:1799:G:H1   | 30:BD:178:PRO:HD2  | 1.79                     | 0.46              |
| 27:BA:1879:C:H2'  | 27:BA:1880:C:C5'   | 2.30                     | 0.46              |
| 27:BA:2277:G:H5'' | 39:BQ:87:LYS:HB2   | 1.98                     | 0.46              |
| 27:BA:2375:G:N2   | 27:BA:2378:A:OP2   | 2.46                     | 0.46              |
| 27:BA:2642:G:C2   | 27:BA:2773:C:C2    | 3.04                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:2767:C:H2'   | 27:BA:2768:C:H6   | 1.80                     | 0.46              |
| 27:BA:2839:G:C4    | 27:BA:2840:C:C5   | 3.03                     | 0.46              |
| 27:BA:293:U:O2     | 27:BA:348:G:C2    | 2.69                     | 0.46              |
| 27:BA:565:C:O2'    | 27:BA:566:U:H5'   | 2.16                     | 0.46              |
| 27:BA:950:G:N2     | 27:BA:968:G:H1'   | 2.31                     | 0.46              |
| 27:BA:96:G:O2'     | 27:BA:97:C:H5'    | 2.15                     | 0.46              |
| 28:BB:35:U:O4      | 28:BB:50:G:H1'    | 2.16                     | 0.46              |
| 30:BD:134:ARG:HG2  | 30:BD:135:PHE:N   | 2.31                     | 0.46              |
| 30:BD:35:LYS:NZ    | 30:BD:102:LYS:C   | 2.68                     | 0.46              |
| 30:BD:72:LYS:HD3   | 30:BD:75:ILE:CD1  | 2.41                     | 0.46              |
| 31:BE:199:ARG:C    | 31:BE:200:GLU:O   | 2.52                     | 0.46              |
| 33:BG:59:GLU:OE1   | 33:BG:153:ARG:NH2 | 2.49                     | 0.46              |
| 33:BG:64:THR:HG23  | 33:BG:66:GLN:H    | 1.80                     | 0.46              |
| 34:BH:103:LEU:HG   | 34:BH:104:GLU:N   | 2.31                     | 0.46              |
| 34:BH:28:GLY:O     | 34:BH:30:LYS:N    | 2.37                     | 0.46              |
| 27:BA:1141:U:P     | 36:BN:25:ARG:NH1  | 2.88                     | 0.46              |
| 36:BN:67:LEU:O     | 36:BN:68:GLU:CG   | 2.57                     | 0.46              |
| 38:BP:16:ARG:HD3   | 38:BP:16:ARG:C    | 2.36                     | 0.46              |
| 38:BP:85:LEU:CD2   | 38:BP:85:LEU:N    | 2.74                     | 0.46              |
| 39:BQ:39:PRO:HD3   | 39:BQ:99:PRO:HG2  | 1.98                     | 0.46              |
| 27:BA:911:A:N6     | 39:BQ:9:TYR:HB3   | 2.30                     | 0.46              |
| 27:BA:2882:A:OP1   | 40:BR:96:ARG:NE   | 2.48                     | 0.46              |
| 42:BT:87:ASP:OD1   | 42:BT:87:ASP:N    | 2.49                     | 0.46              |
| 46:BX:64:LYS:HD3   | 46:BX:73:ARG:NH2  | 2.30                     | 0.46              |
| 47:BY:86:ARG:NH1   | 47:BY:95:LYS:HE2  | 2.31                     | 0.46              |
| 47:BY:96:ILE:CD1   | 47:BY:99:CYS:HB2  | 2.46                     | 0.46              |
| 48:BZ:166:PRO:O    | 48:BZ:167:GLU:HB2 | 2.15                     | 0.46              |
| 48:BZ:172:ALA:O    | 48:BZ:173:VAL:CG2 | 2.63                     | 0.46              |
| 1:CA:117:G:O2'     | 1:CA:118:U:H5'    | 2.16                     | 0.46              |
| 1:CA:1330:U:O3'    | 13:CM:23:TYR:HE2  | 1.99                     | 0.46              |
| 1:CA:945:G:N1      | 1:CA:1337:G:C2    | 2.84                     | 0.46              |
| 1:CA:139:G:O2'     | 1:CA:140:A:H5'    | 2.16                     | 0.46              |
| 1:CA:1442(B):A:H2' | 1:CA:1442(B):A:N3 | 2.31                     | 0.46              |
| 1:CA:22:G:O2'      | 1:CA:23:C:H5'     | 2.16                     | 0.46              |
| 4:CD:206:PHE:CE2   | 4:CD:207:TYR:CE2  | 3.03                     | 0.46              |
| 4:CD:23:GLY:C      | 4:CD:24:GLU:HG2   | 2.36                     | 0.46              |
| 5:CE:6:PHE:H       | 5:CE:6:PHE:HD1    | 1.61                     | 0.46              |
| 8:CH:21:LYS:O      | 8:CH:22:GLU:C     | 2.53                     | 0.46              |
| 9:CI:96:LEU:HG     | 9:CI:102:LEU:HB2  | 1.98                     | 0.46              |
| 9:CI:27:THR:HA     | 9:CI:31:GLN:O     | 2.15                     | 0.46              |
| 14:CN:29:ARG:CG    | 14:CN:40:CYS:HB2  | 2.37                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CP:4:ILE:HB     | 16:CP:66:PRO:HG3   | 1.97                     | 0.46              |
| 17:CQ:51:TYR:CD2   | 17:CQ:73:VAL:HG11  | 2.51                     | 0.46              |
| 24:CX:71:C:H2'     | 24:CX:72:A:O4'     | 2.16                     | 0.46              |
| 25:CY:30:A:C2'     | 25:CY:31:U:H5'     | 2.46                     | 0.46              |
| 49:D0:32:ARG:H     | 49:D0:35:ASN:CG    | 2.19                     | 0.46              |
| 49:D0:37:LEU:HG    | 49:D0:60:PHE:HA    | 1.98                     | 0.46              |
| 49:D0:45:PHE:HZ    | 49:D0:77:ARG:NH1   | 2.14                     | 0.46              |
| 49:D0:56:ASP:OD2   | 49:D0:58:THR:OG1   | 2.33                     | 0.46              |
| 50:D1:90:ILE:H     | 50:D1:90:ILE:HG13  | 1.46                     | 0.46              |
| 55:D6:22:ALA:O     | 55:D6:23:THR:HG23  | 2.16                     | 0.46              |
| 56:D7:46:VAL:CG1   | 56:D7:48:LYS:HZ1   | 2.28                     | 0.46              |
| 27:DA:1260:G:O2'   | 27:DA:1261:C:H5'   | 2.16                     | 0.46              |
| 27:DA:2308:G:H2'   | 27:DA:2309:A:H8    | 1.76                     | 0.46              |
| 27:DA:2393:A:H2'   | 27:DA:2394:C:O4'   | 2.15                     | 0.46              |
| 27:DA:2411:A:H2'   | 27:DA:2412:A:H8    | 1.79                     | 0.46              |
| 27:DA:2552:U:N3    | 27:DA:2554:U:C5'   | 2.78                     | 0.46              |
| 27:DA:2611:U:H3'   | 27:DA:2611:U:OP1   | 2.16                     | 0.46              |
| 27:DA:2818:G:OP2   | 40:DR:42:LYS:NZ    | 2.37                     | 0.46              |
| 27:DA:2893:G:H5'   | 27:DA:2894:G:OP1   | 2.16                     | 0.46              |
| 27:DA:2789:C:N3    | 27:DA:2894:G:O6    | 2.49                     | 0.46              |
| 27:DA:377:C:H2'    | 27:DA:378:C:C6     | 2.46                     | 0.46              |
| 27:DA:476:G:HO2'   | 27:DA:477:A:P      | 2.38                     | 0.46              |
| 27:DA:534:U:H5'    | 43:DU:42:ALA:CB    | 2.45                     | 0.46              |
| 27:DA:610:G:N2     | 27:DA:619:G:HI1'   | 2.31                     | 0.46              |
| 27:DA:675:A:C8     | 27:DA:804:A:N6     | 2.84                     | 0.46              |
| 27:DA:848:G:H2'    | 27:DA:849:A:C8     | 2.51                     | 0.46              |
| 27:DA:84:A:N1      | 27:DA:98:G:H2'     | 2.30                     | 0.46              |
| 28:DB:7:G:H4'      | 41:DS:29:PHE:CD1   | 2.51                     | 0.46              |
| 31:DE:188:VAL:HG22 | 31:DE:189:PRO:CD   | 2.41                     | 0.46              |
| 31:DE:96:PHE:CE2   | 31:DE:198:VAL:HG12 | 2.51                     | 0.46              |
| 31:DE:32:PRO:HA    | 31:DE:90:THR:CA    | 2.46                     | 0.46              |
| 31:DE:92:THR:O     | 31:DE:95:ILE:HD13  | 2.15                     | 0.46              |
| 32:DF:130:ALA:O    | 32:DF:132:VAL:N    | 2.48                     | 0.46              |
| 33:DG:115:ARG:NH1  | 33:DG:136:ARG:HD3  | 2.31                     | 0.46              |
| 33:DG:83:ARG:N     | 33:DG:83:ARG:HD2   | 2.31                     | 0.46              |
| 36:DN:68:GLU:OE1   | 36:DN:68:GLU:HA    | 2.15                     | 0.46              |
| 38:DP:49:ARG:HD2   | 57:D8:58:ILE:HG21  | 1.96                     | 0.46              |
| 39:DQ:110:THR:O    | 39:DQ:113:GLN:HB2  | 2.16                     | 0.46              |
| 39:DQ:20:ALA:O     | 39:DQ:98:LYS:CB    | 2.59                     | 0.46              |
| 40:DR:58:GLY:HA2   | 40:DR:80:PHE:CE1   | 2.51                     | 0.46              |
| 42:DT:12:SER:O     | 42:DT:13:ARG:NH2   | 2.49                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DT:16:ARG:HG3   | 42:DT:16:ARG:NH1   | 2.30                     | 0.46              |
| 42:DT:28:VAL:HG22  | 42:DT:46:GLU:HA    | 1.98                     | 0.46              |
| 42:DT:50:ILE:CG2   | 42:DT:50:ILE:O     | 2.63                     | 0.46              |
| 44:DV:2:PHE:HB3    | 44:DV:42:GLY:HA2   | 1.90                     | 0.46              |
| 48:DZ:156:LEU:HB3  | 48:DZ:160:VAL:O    | 2.16                     | 0.46              |
| 48:DZ:60:LEU:HD23  | 48:DZ:60:LEU:H     | 1.81                     | 0.46              |
| 1:AA:1073:U:H3     | 1:AA:1102:A:N6     | 2.13                     | 0.46              |
| 1:AA:1157:A:O4'    | 1:AA:1158:C:O2     | 2.34                     | 0.46              |
| 1:AA:129:U:H4'     | 1:AA:130:A:OP1     | 2.16                     | 0.46              |
| 1:AA:1360:A:C2'    | 1:AA:1361:G:H5'    | 2.45                     | 0.46              |
| 1:AA:265:G:N2      | 1:AA:267:C:H5'     | 2.31                     | 0.46              |
| 1:AA:293:G:C5      | 1:AA:305:G:N2      | 2.84                     | 0.46              |
| 1:AA:498:U:O2'     | 1:AA:499:A:O5'     | 2.30                     | 0.46              |
| 1:AA:595:G:C6      | 1:AA:641:U:H2'     | 2.50                     | 0.46              |
| 1:AA:689:C:H2'     | 1:AA:690:G:C8      | 2.51                     | 0.46              |
| 1:AA:747:C:H2'     | 1:AA:748:C:O5'     | 2.15                     | 0.46              |
| 1:AA:950:U:H2'     | 1:AA:951:G:H8      | 1.81                     | 0.46              |
| 1:AA:1104:G:H4'    | 2:AB:111:ARG:HD2   | 1.97                     | 0.46              |
| 2:AB:78:GLN:HG2    | 2:AB:94:ASN:HB3    | 1.98                     | 0.46              |
| 4:AD:123:HIS:O     | 4:AD:125:HIS:N     | 2.49                     | 0.46              |
| 6:AF:16:GLN:HE21   | 6:AF:16:GLN:H      | 1.59                     | 0.46              |
| 7:AG:50:ILE:O      | 7:AG:54:THR:O      | 2.33                     | 0.46              |
| 9:AI:96:LEU:CG     | 9:AI:102:LEU:HB2   | 2.46                     | 0.46              |
| 12:AL:44:LYS:CB    | 12:AL:45:PRO:CD    | 2.81                     | 0.46              |
| 14:AN:37:PHE:CE1   | 14:AN:53:LEU:HD13  | 2.51                     | 0.46              |
| 1:AA:741:G:OP1     | 15:AO:35:ARG:NH2   | 2.49                     | 0.46              |
| 16:AP:24:ALA:O     | 16:AP:26:ARG:N     | 2.48                     | 0.46              |
| 16:AP:53:VAL:O     | 16:AP:54:GLU:C     | 2.53                     | 0.46              |
| 24:AX:74:C:O2'     | 24:AX:75:C:H5'     | 2.16                     | 0.46              |
| 50:B1:53:VAL:HG12  | 50:B1:54:ALA:N     | 2.31                     | 0.46              |
| 57:B8:6:THR:CG2    | 57:B8:63:PRO:HD3   | 2.46                     | 0.46              |
| 27:BA:819:A:C4     | 27:BA:1189:A:C2    | 3.04                     | 0.46              |
| 27:BA:1281:G:C6    | 27:BA:1282:U:C4    | 3.03                     | 0.46              |
| 27:BA:1314:C:H42   | 27:BA:1338:G:H1    | 1.63                     | 0.46              |
| 27:BA:1594:G:H5'   | 27:BA:1595:G:OP2   | 2.16                     | 0.46              |
| 27:BA:1741:A:O2'   | 27:BA:1742:G:P     | 2.73                     | 0.46              |
| 27:BA:211:A:H2'    | 27:BA:212:G:H8     | 1.80                     | 0.46              |
| 27:BA:2203:U:O2'   | 27:BA:2205:C:H5'   | 2.15                     | 0.46              |
| 27:BA:2587:A:C2'   | 27:BA:2588:G:H5'   | 2.43                     | 0.46              |
| 27:BA:2023:G:C5'   | 27:BA:2617:C:H4'   | 2.42                     | 0.46              |
| 27:BA:271(K):U:H3' | 27:BA:271(L):U:H5' | 1.97                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2817:G:O2'  | 27:BA:2836:U:O2    | 2.22                     | 0.46              |
| 27:BA:2862:G:C5   | 27:BA:2863:C:C5    | 3.04                     | 0.46              |
| 27:BA:706:A:C8    | 27:BA:707:G:C8     | 3.04                     | 0.46              |
| 27:BA:766:C:C4    | 27:BA:767:U:C4     | 3.04                     | 0.46              |
| 28:BB:107:G:O2'   | 28:BB:108:U:H5'    | 2.15                     | 0.46              |
| 28:BB:40:U:N3     | 28:BB:43:C:C5'     | 2.63                     | 0.46              |
| 30:BD:10:THR:C    | 30:BD:11:PRO:O     | 2.54                     | 0.46              |
| 30:BD:182:LEU:HB3 | 30:BD:271:ILE:HG13 | 1.97                     | 0.46              |
| 30:BD:182:LEU:H   | 30:BD:272:ALA:CB   | 2.25                     | 0.46              |
| 30:BD:173:VAL:O   | 30:BD:184:LYS:HA   | 2.16                     | 0.46              |
| 30:BD:261:LYS:CE  | 30:BD:263:ARG:NH2  | 2.78                     | 0.46              |
| 30:BD:26:LYS:HZ1  | 30:BD:82:ILE:H     | 1.52                     | 0.46              |
| 34:BH:10:PRO:O    | 34:BH:10:PRO:CG    | 2.63                     | 0.46              |
| 35:BI:114:LEU:O   | 35:BI:115:ALA:CB   | 2.63                     | 0.46              |
| 35:BI:5:LEU:HD22  | 35:BI:13:GLY:CA    | 2.33                     | 0.46              |
| 38:BP:79:ARG:NH2  | 38:BP:109:GLY:HA3  | 2.31                     | 0.46              |
| 40:BR:48:VAL:O    | 40:BR:49:ASP:C     | 2.55                     | 0.46              |
| 40:BR:98:LEU:HD12 | 40:BR:113:LEU:CD2  | 2.33                     | 0.46              |
| 42:BT:89:VAL:CG1  | 42:BT:91:ARG:NE    | 2.79                     | 0.46              |
| 47:BY:28:LYS:C    | 47:BY:38:ILE:HB    | 2.34                     | 0.46              |
| 48:BZ:43:PHE:O    | 48:BZ:46:VAL:HB    | 2.16                     | 0.46              |
| 48:BZ:79:ARG:O    | 48:BZ:80:ARG:C     | 2.53                     | 0.46              |
| 1:CA:107:G:OP1    | 1:CA:325:A:N6      | 2.49                     | 0.46              |
| 1:CA:1321:C:H5''  | 1:CA:1322:C:C5'    | 2.31                     | 0.46              |
| 1:CA:1419:G:N3    | 1:CA:1420:C:C6     | 2.84                     | 0.46              |
| 1:CA:230:G:H2'    | 1:CA:231:G:O4'     | 2.16                     | 0.46              |
| 1:CA:447:G:H2'    | 1:CA:485:G:N2      | 2.31                     | 0.46              |
| 1:CA:522:C:H41    | 12:CL:50:ARG:HH22  | 1.62                     | 0.46              |
| 1:CA:738:C:H2'    | 1:CA:739:C:H6      | 1.80                     | 0.46              |
| 1:CA:800:G:O5'    | 1:CA:800:G:H8      | 1.98                     | 0.46              |
| 1:CA:812:C:OP1    | 1:CA:903:G:H1'     | 2.15                     | 0.46              |
| 3:CC:23:TYR:HB2   | 10:CJ:10:GLY:HA2   | 1.98                     | 0.46              |
| 4:CD:150:GLU:HA   | 4:CD:153:ARG:HD2   | 1.97                     | 0.46              |
| 7:CG:41:ARG:O     | 7:CG:42:ILE:C      | 2.54                     | 0.46              |
| 13:CM:47:ASP:O    | 13:CM:48:LEU:CB    | 2.61                     | 0.46              |
| 13:CM:90:LEU:O    | 13:CM:91:ARG:HG2   | 2.16                     | 0.46              |
| 17:CQ:10:VAL:HG11 | 17:CQ:19:VAL:HB    | 1.98                     | 0.46              |
| 49:D0:20:ARG:HH11 | 49:D0:20:ARG:HG3   | 1.69                     | 0.46              |
| 52:D3:11:SER:OG   | 52:D3:13:ILE:HD12  | 2.16                     | 0.46              |
| 52:D3:43:ILE:O    | 52:D3:44:ARG:C     | 2.54                     | 0.46              |
| 52:D3:19:GLN:NE2  | 52:D3:52:HIS:HE1   | 2.13                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:D8:61:LEU:O    | 57:D8:62:LEU:C     | 2.54                     | 0.46              |
| 27:DA:118:A:H1'   | 27:DA:178:G:O4'    | 2.16                     | 0.46              |
| 27:DA:1247:A:O2'  | 27:DA:1248:G:C5'   | 2.64                     | 0.46              |
| 27:DA:1297:C:OP1  | 27:DA:2710:C:H4'   | 2.15                     | 0.46              |
| 27:DA:136:G:H2'   | 27:DA:137:C:H6     | 1.80                     | 0.46              |
| 27:DA:701:G:H4'   | 27:DA:1631(A):A:H2 | 1.81                     | 0.46              |
| 27:DA:1648:C:N3   | 27:DA:2010:G:C2    | 2.84                     | 0.46              |
| 27:DA:1650:G:C4   | 27:DA:1651:G:C8    | 3.04                     | 0.46              |
| 27:DA:186:G:H2'   | 27:DA:187:G:H8     | 1.80                     | 0.46              |
| 27:DA:1697:G:H4'  | 27:DA:1978:A:H5''  | 1.98                     | 0.46              |
| 27:DA:2208:A:H1'  | 27:DA:2219:G:C5    | 2.50                     | 0.46              |
| 27:DA:2241:A:H2'  | 27:DA:2242:G:C8    | 2.51                     | 0.46              |
| 27:DA:2260:C:H6   | 27:DA:2260:C:O5'   | 1.98                     | 0.46              |
| 27:DA:2439:A:H8   | 27:DA:2439:A:C5'   | 2.29                     | 0.46              |
| 27:DA:2523:G:H1'  | 27:DA:2764:A:O2'   | 2.15                     | 0.46              |
| 27:DA:2507:C:H4'  | 27:DA:2573:C:N4    | 2.30                     | 0.46              |
| 27:DA:2807:G:H2'  | 27:DA:2808:U:H5''  | 1.96                     | 0.46              |
| 27:DA:284:U:O2'   | 27:DA:285:C:C5'    | 2.63                     | 0.46              |
| 27:DA:311:A:O2'   | 27:DA:332:A:C5'    | 2.63                     | 0.46              |
| 27:DA:330:A:O2'   | 27:DA:331:A:C8     | 2.57                     | 0.46              |
| 27:DA:459:U:H4'   | 56:D7:40:TRP:CH2   | 2.50                     | 0.46              |
| 27:DA:567:A:C2'   | 27:DA:568:U:O5'    | 2.64                     | 0.46              |
| 27:DA:574:C:O3'   | 27:DA:2055:C:H5    | 1.99                     | 0.46              |
| 27:DA:588:U:H2'   | 27:DA:589:C:C6     | 2.51                     | 0.46              |
| 27:DA:719:C:O2'   | 27:DA:720:C:H5'    | 2.16                     | 0.46              |
| 27:DA:865:C:C4'   | 27:DA:866:A:OP1    | 2.57                     | 0.46              |
| 27:DA:85:G:H1     | 27:DA:97:C:H42     | 1.63                     | 0.46              |
| 30:DD:44:ASN:OD1  | 30:DD:44:ASN:N     | 2.49                     | 0.46              |
| 30:DD:45:ASN:ND2  | 30:DD:50:THR:CG2   | 2.78                     | 0.46              |
| 30:DD:63:ARG:N    | 30:DD:63:ARG:HD3   | 2.30                     | 0.46              |
| 31:DE:2:LYS:O     | 31:DE:199:ARG:CA   | 2.63                     | 0.46              |
| 31:DE:37:ARG:HB2  | 31:DE:46:ALA:HB3   | 1.97                     | 0.46              |
| 32:DF:132:VAL:CG1 | 32:DF:133:ASN:N    | 2.72                     | 0.46              |
| 34:DH:27:LYS:HG2  | 34:DH:32:GLU:CB    | 2.46                     | 0.46              |
| 34:DH:74:ASN:HD22 | 34:DH:74:ASN:H     | 1.62                     | 0.46              |
| 38:DP:18:ARG:HH11 | 38:DP:18:ARG:HB3   | 1.77                     | 0.46              |
| 38:DP:85:LEU:HD23 | 38:DP:115:LEU:O    | 2.15                     | 0.46              |
| 39:DQ:10:ARG:CG   | 39:DQ:10:ARG:NH1   | 2.75                     | 0.46              |
| 40:DR:86:ARG:HB3  | 40:DR:118:GLU:OE2  | 2.15                     | 0.46              |
| 40:DR:47:PHE:O    | 40:DR:47:PHE:CD2   | 2.68                     | 0.46              |
| 42:DT:114:LEU:O   | 42:DT:115:ARG:O    | 2.34                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DT:8:LYS:CA     | 42:DT:11:GLU:OE2   | 2.64                     | 0.46              |
| 44:DV:27:ALA:O     | 44:DV:28:GLU:C     | 2.54                     | 0.46              |
| 44:DV:61:VAL:HA    | 44:DV:94:LEU:CD2   | 2.38                     | 0.46              |
| 45:DW:19:LEU:O     | 45:DW:23:LEU:HD13  | 2.16                     | 0.46              |
| 45:DW:57:ASN:HD22  | 45:DW:57:ASN:HA    | 1.50                     | 0.46              |
| 39:DQ:60:ARG:HG2   | 48:DZ:176:PRO:HB2  | 1.98                     | 0.46              |
| 1:AA:1118:C:H5'    | 1:AA:1118:C:H6     | 1.81                     | 0.46              |
| 1:AA:1200:C:O2'    | 1:AA:1201:A:P      | 2.74                     | 0.46              |
| 1:AA:1494:G:H2'    | 1:AA:1494:G:N3     | 2.31                     | 0.46              |
| 1:AA:578:C:O2'     | 1:AA:579:G:P       | 2.74                     | 0.46              |
| 1:AA:916:G:C2      | 1:AA:917:G:C8      | 3.04                     | 0.46              |
| 2:AB:141:GLU:O     | 2:AB:145:LEU:HB2   | 2.16                     | 0.46              |
| 2:AB:236:TYR:HD1   | 2:AB:236:TYR:N     | 2.13                     | 0.46              |
| 2:AB:53:ARG:NH2    | 2:AB:199:TYR:CE2   | 2.84                     | 0.46              |
| 6:AF:62:TRP:CD1    | 18:AR:35:ARG:CZ    | 2.99                     | 0.46              |
| 9:AI:48:GLU:HB2    | 9:AI:78:LYS:HZ1    | 1.80                     | 0.46              |
| 13:AM:83:ASP:O     | 13:AM:85:GLY:N     | 2.48                     | 0.46              |
| 1:AA:230:G:H5'     | 16:AP:23:ASP:OD2   | 2.16                     | 0.46              |
| 49:B0:56:ASP:O     | 49:B0:57:PHE:CB    | 2.62                     | 0.46              |
| 50:B1:64:ALA:HA    | 50:B1:67:ILE:HD12  | 1.97                     | 0.46              |
| 53:B4:44:CYS:HB2   | 53:B4:64:LYS:HD2   | 1.97                     | 0.46              |
| 27:BA:2358:G:H21   | 57:B8:52:LYS:HE2   | 1.80                     | 0.46              |
| 27:BA:139:G:C4     | 27:BA:140:G:N7     | 2.84                     | 0.46              |
| 27:BA:1603:A:H3'   | 27:BA:1604:C:H6    | 1.80                     | 0.46              |
| 27:BA:1806:C:O2'   | 27:BA:1807:G:H5'   | 2.15                     | 0.46              |
| 27:BA:1827:C:N4    | 27:BA:1828:G:C6    | 2.84                     | 0.46              |
| 27:BA:2129:C:N3    | 27:BA:2160:G:C6    | 2.84                     | 0.46              |
| 27:BA:2453:A:H2'   | 27:BA:2454:G:C8    | 2.51                     | 0.46              |
| 27:BA:252:G:OP2    | 38:BP:50:ARG:NH1   | 2.48                     | 0.46              |
| 27:BA:271(I):G:H2' | 27:BA:271(J):C:C1' | 2.46                     | 0.46              |
| 27:BA:2863:C:O2    | 27:BA:2863:C:H2'   | 2.15                     | 0.46              |
| 27:BA:310:A:C4     | 27:BA:312:G:C8     | 3.04                     | 0.46              |
| 27:BA:34:C:HO2'    | 27:BA:35:G:H5'     | 1.78                     | 0.46              |
| 27:BA:807:U:O2'    | 27:BA:808:G:C5'    | 2.52                     | 0.46              |
| 27:BA:845:G:O2'    | 27:BA:846:C:C6     | 2.66                     | 0.46              |
| 27:BA:93:G:H2'     | 27:BA:94:C:C6      | 2.51                     | 0.46              |
| 28:BB:28:C:H2'     | 28:BB:29:A:O4'     | 2.16                     | 0.46              |
| 28:BB:70:C:H2'     | 28:BB:71:C:H6      | 1.81                     | 0.46              |
| 30:BD:248:SER:O    | 30:BD:250:TRP:N    | 2.49                     | 0.46              |
| 30:BD:271:ILE:O    | 30:BD:272:ALA:HB2  | 2.16                     | 0.46              |
| 30:BD:182:LEU:N    | 30:BD:272:ALA:HB3  | 2.27                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:674:G:H1'   | 32:BF:74:ARG:HD3  | 1.98                     | 0.46              |
| 33:BG:21:ARG:CD   | 33:BG:21:ARG:C    | 2.84                     | 0.46              |
| 27:BA:2310:A:H62  | 33:BG:75:LYS:NZ   | 2.14                     | 0.46              |
| 34:BH:26:VAL:O    | 34:BH:26:VAL:HG12 | 2.16                     | 0.46              |
| 34:BH:38:SER:C    | 34:BH:40:GLU:N    | 2.69                     | 0.46              |
| 34:BH:8:PRO:HD3   | 34:BH:65:HIS:HE1  | 1.81                     | 0.46              |
| 36:BN:32:THR:O    | 36:BN:35:ARG:O    | 2.34                     | 0.46              |
| 38:BP:105:LEU:O   | 38:BP:106:LEU:CB  | 2.62                     | 0.46              |
| 41:BS:97:ARG:NE   | 41:BS:98:VAL:N    | 2.58                     | 0.46              |
| 42:BT:35:LYS:C    | 42:BT:37:GLY:N    | 2.69                     | 0.46              |
| 43:BU:12:ARG:O    | 43:BU:13:LYS:C    | 2.54                     | 0.46              |
| 44:BV:19:LYS:NZ   | 44:BV:20:LEU:HB2  | 2.31                     | 0.46              |
| 27:BA:2010:G:C5'  | 45:BW:42:ARG:HB2  | 2.46                     | 0.46              |
| 45:BW:57:ASN:N    | 45:BW:57:ASN:ND2  | 2.63                     | 0.46              |
| 47:BY:6:HIS:HB2   | 47:BY:7:VAL:H     | 1.54                     | 0.46              |
| 48:BZ:150:HIS:O   | 48:BZ:151:ALA:O   | 2.34                     | 0.46              |
| 1:CA:1059:C:O2'   | 1:CA:1060:C:H5'   | 2.16                     | 0.46              |
| 1:CA:1336:C:H4'   | 1:CA:1337:G:C4    | 2.51                     | 0.46              |
| 1:CA:197:A:N6     | 1:CA:221:C:C5'    | 2.75                     | 0.46              |
| 1:CA:563:A:HO2'   | 1:CA:567:G:H8     | 1.61                     | 0.46              |
| 1:CA:694:A:H2'    | 1:CA:695:A:O4'    | 2.15                     | 0.46              |
| 1:CA:718:G:H21    | 18:CR:49:LYS:HZ2  | 1.60                     | 0.46              |
| 1:CA:760:G:H3'    | 1:CA:761:G:H8     | 1.81                     | 0.46              |
| 1:CA:836:G:H2'    | 1:CA:837:G:C8     | 2.51                     | 0.46              |
| 3:CC:150:LYS:HD3  | 3:CC:201:TYR:CD1  | 2.40                     | 0.46              |
| 4:CD:155:LEU:HB2  | 4:CD:158:ILE:HG12 | 1.98                     | 0.46              |
| 6:CF:38:GLU:O     | 6:CF:39:LYS:CB    | 2.49                     | 0.46              |
| 7:CG:153:HIS:N    | 7:CG:153:HIS:ND1  | 2.64                     | 0.46              |
| 8:CH:89:PRO:HA    | 8:CH:92:ARG:NH1   | 2.31                     | 0.46              |
| 1:CA:972:C:H4'    | 10:CJ:57:LYS:HG3  | 1.96                     | 0.46              |
| 11:CK:60:ALA:O    | 11:CK:63:LEU:N    | 2.49                     | 0.46              |
| 13:CM:29:ARG:HB3  | 13:CM:64:TRP:CH2  | 2.51                     | 0.46              |
| 13:CM:88:ARG:HG3  | 13:CM:98:VAL:CG1  | 2.46                     | 0.46              |
| 20:CT:14:LYS:CB   | 20:CT:17:ARG:HH21 | 2.16                     | 0.46              |
| 23:CW:16:C:O5'    | 23:CW:16:C:H6     | 1.98                     | 0.46              |
| 24:CX:59:A:H2'    | 24:CX:60:U:H5'    | 1.98                     | 0.46              |
| 51:D2:65:ASN:HB3  | 51:D2:69:ARG:HH22 | 1.81                     | 0.46              |
| 57:D8:51:ALA:HA   | 57:D8:54:GLU:OE2  | 2.15                     | 0.46              |
| 57:D8:61:LEU:HD12 | 57:D8:62:LEU:H    | 1.79                     | 0.46              |
| 58:D9:17:ILE:HG22 | 58:D9:19:ARG:H    | 1.80                     | 0.46              |
| 27:DA:1419:A:H2'  | 27:DA:1421:G:C5   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:1558:A:H4'  | 27:DA:1559:G:O5'  | 2.15                     | 0.46              |
| 27:DA:1674:G:H5'  | 27:DA:1675:C:OP1  | 2.16                     | 0.46              |
| 27:DA:1882:C:H2'  | 27:DA:1882:C:O2   | 2.15                     | 0.46              |
| 27:DA:1893:C:H2'  | 27:DA:1894:C:H6   | 1.81                     | 0.46              |
| 27:DA:2235:G:N2   | 27:DA:2236:C:C2   | 2.84                     | 0.46              |
| 27:DA:2582:G:H2'  | 27:DA:2583:G:O4'  | 2.15                     | 0.46              |
| 27:DA:2791:C:H1'  | 27:DA:2792:G:C8   | 2.51                     | 0.46              |
| 27:DA:2884:U:H2'  | 27:DA:2885:C:C5'  | 2.42                     | 0.46              |
| 28:DB:25:A:C3'    | 28:DB:26:A:H5''   | 2.46                     | 0.46              |
| 28:DB:25:A:H5'    | 28:DB:25:A:C8     | 2.51                     | 0.46              |
| 28:DB:87:G:H1     | 28:DB:91:C:N4     | 2.13                     | 0.46              |
| 33:DG:59:GLU:O    | 33:DG:62:LEU:HB2  | 2.16                     | 0.46              |
| 33:DG:5:VAL:CG2   | 33:DG:8:LYS:HG3   | 2.35                     | 0.46              |
| 34:DH:126:PRO:O   | 34:DH:127:GLU:CB  | 2.54                     | 0.46              |
| 34:DH:135:GLY:HA3 | 34:DH:141:VAL:CG2 | 2.46                     | 0.46              |
| 34:DH:13:LYS:HE2  | 34:DH:13:LYS:CA   | 2.39                     | 0.46              |
| 37:DO:36:GLY:HA2  | 37:DO:106:LEU:CD2 | 2.46                     | 0.46              |
| 32:DF:187:VAL:CB  | 38:DP:7:ARG:NH2   | 2.77                     | 0.46              |
| 39:DQ:29:PHE:O    | 39:DQ:30:GLY:O    | 2.34                     | 0.46              |
| 40:DR:18:LEU:HD11 | 40:DR:22:ARG:NH1  | 2.30                     | 0.46              |
| 41:DS:27:SER:HA   | 41:DS:88:ASP:HB3  | 1.98                     | 0.46              |
| 41:DS:69:VAL:O    | 41:DS:72:ALA:N    | 2.49                     | 0.46              |
| 42:DT:129:ARG:HD2 | 42:DT:131:ALA:CB  | 2.46                     | 0.46              |
| 42:DT:2:ASN:O     | 42:DT:3:ARG:CD    | 2.63                     | 0.46              |
| 44:DV:38:LEU:CD1  | 44:DV:55:ALA:HB1  | 2.46                     | 0.46              |
| 1:AA:1183:A:H3'   | 1:AA:1184:G:H5''  | 1.98                     | 0.46              |
| 1:AA:494:U:C6     | 1:AA:494:U:O5'    | 2.69                     | 0.46              |
| 1:AA:741:G:O2'    | 1:AA:742:G:H5'    | 2.16                     | 0.46              |
| 4:AD:166:LYS:HD3  | 4:AD:179:GLU:OE2  | 2.16                     | 0.46              |
| 7:AG:11:GLN:O     | 7:AG:12:LEU:HG    | 2.15                     | 0.46              |
| 7:AG:18:TYR:O     | 7:AG:19:GLY:C     | 2.54                     | 0.46              |
| 8:AH:65:TYR:HA    | 8:AH:79:VAL:HG23  | 1.97                     | 0.46              |
| 12:AL:73:ASN:O    | 12:AL:74:LEU:C    | 2.54                     | 0.46              |
| 13:AM:96:LEU:HD21 | 13:AM:111:LYS:HD2 | 1.98                     | 0.46              |
| 15:AO:74:ASP:OD2  | 15:AO:77:ARG:N    | 2.32                     | 0.46              |
| 19:AS:47:HIS:O    | 19:AS:62:ILE:HG21 | 2.15                     | 0.46              |
| 49:B0:50:ASN:HB2  | 49:B0:81:VAL:HB   | 1.98                     | 0.46              |
| 55:B6:41:PRO:HD2  | 55:B6:46:HIS:N    | 2.30                     | 0.46              |
| 56:B7:8:ASN:HD22  | 56:B7:9:ARG:N     | 2.10                     | 0.46              |
| 27:BA:1322:A:C5   | 27:BA:1323:U:C5   | 3.04                     | 0.46              |
| 27:BA:1416:G:HO2' | 27:BA:1417:C:H6   | 1.60                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 27:BA:1632:A:C6     | 27:BA:1633:G:C6    | 3.04                     | 0.46              |
| 27:BA:1698:A:O4'    | 27:BA:1700:A:C4'   | 2.64                     | 0.46              |
| 27:BA:2176:A:H2'    | 27:BA:2177:C:C6    | 2.51                     | 0.46              |
| 27:BA:2367:G:H2'    | 27:BA:2368:C:H6    | 1.81                     | 0.46              |
| 27:BA:2448:A:OP1    | 27:BA:2499:C:OP1   | 2.34                     | 0.46              |
| 27:BA:2646:C:H2'    | 27:BA:2647:U:H6    | 1.80                     | 0.46              |
| 27:BA:2692:C:H2'    | 27:BA:2693:A:H8    | 1.81                     | 0.46              |
| 27:BA:271(O):C:HO2' | 27:BA:271(P):C:H5  | 1.61                     | 0.46              |
| 27:BA:2844:G:C2'    | 27:BA:2845:G:H5'   | 2.46                     | 0.46              |
| 27:BA:2848:G:H1'    | 27:BA:2868:A:N6    | 2.30                     | 0.46              |
| 27:BA:299:A:C5      | 27:BA:322:A:C2     | 3.04                     | 0.46              |
| 27:BA:340:A:H2'     | 27:BA:341:G:O5'    | 2.16                     | 0.46              |
| 27:BA:70:G:H2'      | 27:BA:113:G:O2'    | 2.15                     | 0.46              |
| 27:BA:745:G:O2'     | 27:BA:750:A:N6     | 2.49                     | 0.46              |
| 27:BA:782:A:H4'     | 27:BA:783:A:O5'    | 2.17                     | 0.46              |
| 27:BA:828:U:H4'     | 27:BA:831:G:H1     | 1.79                     | 0.46              |
| 27:BA:893:C:H2'     | 27:BA:894:C:O4'    | 2.15                     | 0.46              |
| 27:BA:996:A:O2'     | 27:BA:997:G:O5'    | 2.32                     | 0.46              |
| 30:BD:31:LYS:NZ     | 30:BD:102:LYS:HZ3  | 2.14                     | 0.46              |
| 30:BD:186:HIS:CD2   | 30:BD:188:GLU:CG   | 2.99                     | 0.46              |
| 30:BD:132:PRO:HD3   | 30:BD:190:TYR:CE2  | 2.51                     | 0.46              |
| 30:BD:218:ARG:HB3   | 30:BD:219:PRO:HD2  | 1.98                     | 0.46              |
| 31:BE:120:TRP:CD1   | 31:BE:155:LYS:HB3  | 2.51                     | 0.46              |
| 35:BI:38:LEU:N      | 35:BI:38:LEU:HD12  | 2.17                     | 0.46              |
| 36:BN:134:ARG:O     | 36:BN:135:PRO:C    | 2.53                     | 0.46              |
| 36:BN:43:THR:HB     | 36:BN:46:VAL:HG12  | 1.97                     | 0.46              |
| 37:BO:4:PRO:O       | 37:BO:5:GLN:HB2    | 2.16                     | 0.46              |
| 38:BP:114:ILE:O     | 38:BP:115:LEU:HB3  | 2.16                     | 0.46              |
| 38:BP:59:LEU:CA     | 38:BP:61:ARG:NH1   | 2.70                     | 0.46              |
| 44:BV:39:LEU:CA     | 44:BV:47:VAL:HG11  | 2.45                     | 0.46              |
| 48:BZ:47:PHE:CD1    | 48:BZ:51:SER:HA    | 2.51                     | 0.46              |
| 1:CA:1030(A):G:H3'  | 1:CA:1030(B):C:C5' | 2.46                     | 0.46              |
| 1:CA:1049:U:O2'     | 1:CA:1050:G:P      | 2.74                     | 0.46              |
| 1:CA:1126:U:C2'     | 1:CA:1127:G:O5'    | 2.64                     | 0.46              |
| 1:CA:1054:C:C5      | 1:CA:1196:U:H2'    | 2.50                     | 0.46              |
| 1:CA:1232:U:C4      | 1:CA:1233:G:N7     | 2.84                     | 0.46              |
| 1:CA:134:A:C6       | 1:CA:135:C:N3      | 2.84                     | 0.46              |
| 1:CA:1466:C:C2'     | 1:CA:1467:G:H5'    | 2.45                     | 0.46              |
| 1:CA:578:C:O2'      | 1:CA:579:G:H5'     | 2.16                     | 0.46              |
| 1:CA:601:C:C2       | 1:CA:602:A:C8      | 3.04                     | 0.46              |
| 1:CA:781:A:H4'      | 1:CA:1522:U:O2'    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:187:LEU:C    | 2:CB:187:LEU:HD22  | 2.36                     | 0.46              |
| 6:CF:17:SER:O     | 6:CF:21:LEU:HD23   | 2.16                     | 0.46              |
| 9:CI:8:GLY:O      | 9:CI:14:VAL:HA     | 2.16                     | 0.46              |
| 11:CK:17:GLY:O    | 11:CK:80:VAL:HA    | 2.16                     | 0.46              |
| 12:CL:43:LYS:HD3  | 12:CL:44:LYS:HG2   | 1.98                     | 0.46              |
| 12:CL:4:ILE:O     | 12:CL:7:LEU:N      | 2.49                     | 0.46              |
| 1:CA:947:G:H4'    | 13:CM:109:THR:OG1  | 2.16                     | 0.46              |
| 17:CQ:12:SER:HB3  | 17:CQ:20:THR:CB    | 2.46                     | 0.46              |
| 20:CT:16:HIS:O    | 20:CT:19:SER:HB3   | 2.15                     | 0.46              |
| 24:CX:38:A:H2'    | 24:CX:39:C:H6      | 1.80                     | 0.46              |
| 25:CY:38:U:O2     | 25:CY:38:U:C3'     | 2.64                     | 0.46              |
| 51:D2:4:SER:O     | 51:D2:7:ARG:HG3    | 2.16                     | 0.46              |
| 27:DA:1170:G:N2   | 27:DA:1180:C:C4    | 2.83                     | 0.46              |
| 27:DA:52:A:C5     | 27:DA:118:A:C2     | 3.04                     | 0.46              |
| 27:DA:1482:G:H22  | 27:DA:1507:A:H1'   | 1.80                     | 0.46              |
| 27:DA:1718:G:O2'  | 27:DA:1719:G:H5'   | 2.15                     | 0.46              |
| 27:DA:2189:U:H2'  | 27:DA:2189:U:O2    | 2.16                     | 0.46              |
| 27:DA:2248:C:H5'' | 27:DA:2249:U:OP2   | 2.15                     | 0.46              |
| 27:DA:631:A:H2    | 27:DA:2403:C:O2    | 1.99                     | 0.46              |
| 27:DA:30:G:H4'    | 27:DA:1215:G:H5'   | 1.98                     | 0.46              |
| 27:DA:483:A:H1'   | 47:DY:60:PHE:CZ    | 2.51                     | 0.46              |
| 27:DA:620:G:C4'   | 27:DA:621:A:OP1    | 2.63                     | 0.46              |
| 27:DA:84:A:N1     | 27:DA:98:G:O2'     | 2.41                     | 0.46              |
| 27:DA:878:A:N6    | 27:DA:899:A:O2'    | 2.48                     | 0.46              |
| 27:DA:969:U:P     | 52:D3:17:LYS:NZ    | 2.89                     | 0.46              |
| 30:DD:264:LYS:HA  | 30:DD:265:PRO:HD3  | 1.79                     | 0.46              |
| 30:DD:45:ASN:CG   | 30:DD:46:GLN:H     | 2.19                     | 0.46              |
| 32:DF:20:LEU:HB3  | 32:DF:23:ASP:OD2   | 2.16                     | 0.46              |
| 27:DA:674:G:H1'   | 32:DF:74:ARG:HD3   | 1.97                     | 0.46              |
| 32:DF:8:GLN:NE2   | 32:DF:9:ILE:HG13   | 2.31                     | 0.46              |
| 32:DF:99:TYR:CD2  | 32:DF:99:TYR:C     | 2.90                     | 0.46              |
| 35:DI:58:LEU:C    | 35:DI:60:GLU:N     | 2.70                     | 0.46              |
| 38:DP:110:TYR:HE2 | 38:DP:111:ARG:HH21 | 1.64                     | 0.46              |
| 38:DP:140:ALA:O   | 38:DP:141:ALA:CB   | 2.64                     | 0.46              |
| 39:DQ:61:GLY:O    | 39:DQ:62:GLY:O     | 2.34                     | 0.46              |
| 39:DQ:61:GLY:O    | 39:DQ:62:GLY:C     | 2.54                     | 0.46              |
| 41:DS:30:ARG:NH1  | 41:DS:34:HIS:O     | 2.49                     | 0.46              |
| 43:DU:60:LEU:HA   | 43:DU:63:VAL:HG23  | 1.98                     | 0.46              |
| 44:DV:35:LEU:HB2  | 44:DV:57:VAL:HG13  | 1.98                     | 0.46              |
| 45:DW:10:VAL:O    | 45:DW:11:ARG:CB    | 2.63                     | 0.46              |
| 45:DW:65:LEU:HD13 | 45:DW:68:ARG:CG    | 2.46                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 47:DY:7:VAL:HG21 | 47:DY:8:LYS:HZ3    | 1.81                     | 0.46              |
| 47:DY:96:ILE:CD1 | 47:DY:99:CYS:HB2   | 2.46                     | 0.46              |
| 48:DZ:149:LEU:N  | 48:DZ:149:LEU:HD13 | 2.31                     | 0.46              |
| 1:AA:920:U:H1'   | 1:AA:1080:A:N3     | 2.31                     | 0.45              |
| 1:AA:1145:C:H4'  | 1:AA:1146:A:OP1    | 2.15                     | 0.45              |
| 1:AA:1355:G:H2'  | 1:AA:1356:G:C8     | 2.51                     | 0.45              |
| 1:AA:1355:G:O2'  | 1:AA:1356:G:H5'    | 2.16                     | 0.45              |
| 1:AA:155:C:O2    | 1:AA:167:G:C2      | 2.69                     | 0.45              |
| 1:AA:172:A:N7    | 1:AA:174:C:C4      | 2.84                     | 0.45              |
| 1:AA:247:G:O6    | 1:AA:278:G:C6      | 2.69                     | 0.45              |
| 1:AA:577:G:C2    | 1:AA:578:C:C5      | 3.03                     | 0.45              |
| 1:AA:814:A:N7    | 1:AA:816:A:C5      | 2.84                     | 0.45              |
| 1:AA:839:U:O2    | 1:AA:839:U:H2'     | 2.16                     | 0.45              |
| 1:AA:960:U:O2'   | 1:AA:1223:C:H4'    | 2.16                     | 0.45              |
| 2:AB:57:PHE:CE2  | 2:AB:185:ILE:HD11  | 2.50                     | 0.45              |
| 2:AB:81:VAL:O    | 2:AB:85:ALA:HB2    | 2.16                     | 0.45              |
| 3:AC:182:ILE:CG1 | 3:AC:203:PHE:HD1   | 2.29                     | 0.45              |
| 4:AD:17:VAL:CG1  | 4:AD:197:PRO:HG3   | 2.31                     | 0.45              |
| 9:AI:19:LEU:HB3  | 9:AI:59:PHE:CD2    | 2.51                     | 0.45              |
| 10:AJ:3:LYS:HB2  | 10:AJ:77:PRO:CG    | 2.46                     | 0.45              |
| 13:AM:66:LEU:O   | 13:AM:67:GLU:C     | 2.53                     | 0.45              |
| 16:AP:14:ASN:N   | 16:AP:15:PRO:CD    | 2.68                     | 0.45              |
| 23:AW:44:A:O2'   | 23:AW:45:U:OP1     | 2.29                     | 0.45              |
| 23:AW:4:G:C2'    | 23:AW:5:G:H5''     | 2.45                     | 0.45              |
| 25:AY:24:C:H2'   | 25:AY:25:A:H8      | 1.80                     | 0.45              |
| 50:B1:19:GLN:N   | 50:B1:36:GLY:O     | 2.48                     | 0.45              |
| 58:B9:27:CYS:SG  | 58:B9:32:HIS:CB    | 3.05                     | 0.45              |
| 27:BA:1010:A:H8  | 27:BA:1010:A:O5'   | 1.98                     | 0.45              |
| 27:BA:1188:U:H4' | 44:BV:79:VAL:HG22  | 1.97                     | 0.45              |
| 27:BA:1310:G:C2  | 27:BA:1313:U:O4    | 2.69                     | 0.45              |
| 27:BA:1333:C:H2' | 27:BA:1334:G:C8    | 2.51                     | 0.45              |
| 27:BA:1668:A:C8  | 27:BA:1674:G:C5    | 3.04                     | 0.45              |
| 27:BA:1782:C:C4  | 27:BA:2587:A:C2    | 3.04                     | 0.45              |
| 27:BA:1783:A:N1  | 27:BA:2587:A:C4    | 2.84                     | 0.45              |
| 27:BA:1923:U:H2' | 27:BA:1924:C:H6    | 1.82                     | 0.45              |
| 27:BA:2111:C:OP2 | 27:BA:2111:C:C6    | 2.69                     | 0.45              |
| 27:BA:2384:G:OP1 | 49:B0:55:ARG:NH1   | 2.49                     | 0.45              |
| 27:BA:2439:A:C5' | 27:BA:2439:A:H8    | 2.24                     | 0.45              |
| 27:BA:792:G:O2'  | 27:BA:2440:C:N3    | 2.42                     | 0.45              |
| 27:BA:2459:A:H5' | 27:BA:2460:U:OP2   | 2.16                     | 0.45              |
| 27:BA:2720:U:O4  | 27:BA:2873:A:N7    | 2.49                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:36:G:N1      | 27:BA:445:C:C4     | 2.84                     | 0.45              |
| 27:BA:563:G:N1     | 27:BA:564:C:C4     | 2.84                     | 0.45              |
| 27:BA:636:G:P      | 38:BP:131:SER:HB2  | 2.55                     | 0.45              |
| 27:BA:705:A:C2     | 27:BA:727:A:H1'    | 2.51                     | 0.45              |
| 27:BA:940:G:N2     | 27:BA:941:A:C4     | 2.84                     | 0.45              |
| 28:BB:29:A:H2'     | 28:BB:30:C:H6      | 1.80                     | 0.45              |
| 30:BD:201:HIS:C    | 30:BD:201:HIS:ND1  | 2.68                     | 0.45              |
| 31:BE:130:GLY:C    | 31:BE:131:ALA:O    | 2.55                     | 0.45              |
| 32:BF:192:LEU:HD21 | 32:BF:194:MET:HG2  | 1.99                     | 0.45              |
| 33:BG:167:GLU:O    | 33:BG:168:GLU:C    | 2.55                     | 0.45              |
| 36:BN:58:ASP:C     | 36:BN:60:ILE:N     | 2.70                     | 0.45              |
| 36:BN:76:SER:O     | 36:BN:78:TYR:HD1   | 1.99                     | 0.45              |
| 27:BA:2484:G:O2'   | 39:BQ:124:LYS:O    | 2.34                     | 0.45              |
| 39:BQ:16:ARG:C     | 39:BQ:17:LEU:HD23  | 2.36                     | 0.45              |
| 40:BR:19:ALA:O     | 40:BR:23:ASN:ND2   | 2.49                     | 0.45              |
| 41:BS:74:ALA:O     | 41:BS:77:ALA:HB3   | 2.16                     | 0.45              |
| 41:BS:97:ARG:CZ    | 41:BS:98:VAL:HA    | 2.38                     | 0.45              |
| 42:BT:82:LEU:N     | 42:BT:82:LEU:HD12  | 2.31                     | 0.45              |
| 44:BV:87:HIS:C     | 44:BV:87:HIS:CD2   | 2.89                     | 0.45              |
| 1:CA:1016:A:H8     | 1:CA:1016:A:O5'    | 2.00                     | 0.45              |
| 1:CA:1057:G:C2'    | 1:CA:1058:G:O5'    | 2.64                     | 0.45              |
| 1:CA:1162:C:H2'    | 1:CA:1163:C:C6     | 2.51                     | 0.45              |
| 1:CA:1168:A:OP1    | 1:CA:1168:A:H8     | 1.99                     | 0.45              |
| 1:CA:1209:C:C2'    | 1:CA:1210:C:H5'    | 2.45                     | 0.45              |
| 1:CA:971:G:N2      | 1:CA:1363(A):A:OP2 | 2.38                     | 0.45              |
| 1:CA:144:G:N2      | 1:CA:178:C:O2      | 2.49                     | 0.45              |
| 1:CA:460:G:C8      | 1:CA:460:G:O5'     | 2.69                     | 0.45              |
| 1:CA:736:C:H2'     | 1:CA:737:A:C8      | 2.51                     | 0.45              |
| 1:CA:862:C:H1'     | 1:CA:874:G:C5'     | 2.46                     | 0.45              |
| 1:CA:965:A:H5''    | 1:CA:966:G:OP1     | 2.15                     | 0.45              |
| 5:CE:80:ILE:CD1    | 5:CE:91:LEU:HB2    | 2.45                     | 0.45              |
| 8:CH:71:GLY:O      | 8:CH:73:ASP:N      | 2.49                     | 0.45              |
| 17:CQ:53:LEU:HD12  | 17:CQ:54:GLY:N     | 2.31                     | 0.45              |
| 19:CS:63:THR:HG22  | 19:CS:66:MET:HE2   | 1.98                     | 0.45              |
| 20:CT:80:ARG:O     | 20:CT:84:LEU:N     | 2.49                     | 0.45              |
| 23:CW:1:U:P        | 23:CW:1:U:H6       | 2.39                     | 0.45              |
| 50:D1:95:LEU:HD12  | 50:D1:95:LEU:HA    | 1.80                     | 0.45              |
| 52:D3:18:ASP:N     | 52:D3:18:ASP:OD1   | 2.48                     | 0.45              |
| 27:DA:2056:G:H1    | 54:D5:4:HIS:HD2    | 1.64                     | 0.45              |
| 27:DA:991:C:C2     | 27:DA:1164:G:C2    | 3.05                     | 0.45              |
| 27:DA:52:A:N6      | 27:DA:118:A:C4     | 2.84                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1410:G:H2'   | 27:DA:1411:C:C5    | 2.47                     | 0.45              |
| 27:DA:153:C:OP1    | 50:D1:92:LYS:NZ    | 2.44                     | 0.45              |
| 1:CA:1484:C:H4'    | 27:DA:1960:A:O2'   | 2.16                     | 0.45              |
| 27:DA:2197:U:HO2'  | 27:DA:2198:A:P     | 2.39                     | 0.45              |
| 27:DA:2266:A:H5''  | 27:DA:2267:A:O5'   | 2.16                     | 0.45              |
| 27:DA:258:G:H2'    | 27:DA:259:G:H8     | 1.81                     | 0.45              |
| 27:DA:27:G:O2'     | 27:DA:28:A:H8      | 1.99                     | 0.45              |
| 27:DA:283:A:C2     | 27:DA:427:U:H1'    | 2.50                     | 0.45              |
| 27:DA:763:G:C8     | 27:DA:763:G:H3'    | 2.50                     | 0.45              |
| 27:DA:845:G:C8     | 27:DA:845:G:C5'    | 2.99                     | 0.45              |
| 28:DB:24:G:H1'     | 28:DB:27:C:N4      | 2.31                     | 0.45              |
| 29:DC:48:GLY:O     | 29:DC:49:ILE:O     | 2.34                     | 0.45              |
| 30:DD:190:TYR:O    | 30:DD:191:ALA:HB2  | 2.16                     | 0.45              |
| 30:DD:69:ARG:HG2   | 30:DD:69:ARG:O     | 2.16                     | 0.45              |
| 31:DE:116:VAL:CG2  | 31:DE:122:PHE:CG   | 2.98                     | 0.45              |
| 31:DE:9:VAL:HG22   | 42:DT:8:LYS:HD2    | 1.98                     | 0.45              |
| 33:DG:114:ILE:CG2  | 33:DG:115:ARG:N    | 2.80                     | 0.45              |
| 33:DG:99:MET:O     | 33:DG:103:LEU:HD12 | 2.16                     | 0.45              |
| 34:DH:119:GLU:O    | 34:DH:140:LYS:NZ   | 2.47                     | 0.45              |
| 35:DI:88:ILE:O     | 35:DI:89:TYR:C     | 2.52                     | 0.45              |
| 37:DO:10:VAL:HG13  | 37:DO:17:ARG:C     | 2.36                     | 0.45              |
| 37:DO:116:SER:C    | 37:DO:118:ALA:H    | 2.17                     | 0.45              |
| 38:DP:24:GLY:O     | 38:DP:25:SER:HB3   | 2.17                     | 0.45              |
| 39:DQ:98:LYS:CB    | 39:DQ:99:PRO:CD    | 2.92                     | 0.45              |
| 41:DS:14:VAL:HG12  | 41:DS:15:ARG:N     | 2.31                     | 0.45              |
| 41:DS:34:HIS:ND1   | 41:DS:54:LEU:HB2   | 2.29                     | 0.45              |
| 27:DA:18:C:O2'     | 43:DU:23:GLY:HA2   | 2.16                     | 0.45              |
| 44:DV:16:PRO:O     | 44:DV:96:ILE:HB    | 2.17                     | 0.45              |
| 44:DV:34:GLU:O     | 44:DV:36:PRO:N     | 2.49                     | 0.45              |
| 45:DW:92:ARG:NH1   | 45:DW:94:ASP:OD2   | 2.49                     | 0.45              |
| 1:AA:1030(C):G:O2' | 1:AA:1030(D):A:H5' | 2.16                     | 0.45              |
| 1:AA:1097:C:H1'    | 1:AA:1170:A:H1'    | 1.97                     | 0.45              |
| 1:AA:1166:G:H2'    | 1:AA:1169:A:OP2    | 2.16                     | 0.45              |
| 1:AA:1226:C:N4     | 13:AM:104:ARG:HD3  | 2.32                     | 0.45              |
| 1:AA:1363(A):A:C4  | 1:AA:1365:G:C6     | 3.04                     | 0.45              |
| 1:AA:1376:U:O4     | 7:AG:10:ARG:NH2    | 2.46                     | 0.45              |
| 1:AA:129(A):G:O6   | 1:AA:189(D):C:O2'  | 2.34                     | 0.45              |
| 1:AA:262:A:H2'     | 1:AA:263:A:C8      | 2.51                     | 0.45              |
| 1:AA:279:A:O2'     | 1:AA:280:C:OP2     | 2.29                     | 0.45              |
| 1:AA:355:C:H5'     | 1:AA:389:A:OP2     | 2.16                     | 0.45              |
| 1:AA:404:U:O2'     | 1:AA:405:U:H5'     | 2.16                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:455:C:H2'    | 1:AA:456:C:H5'     | 1.97                     | 0.45              |
| 1:AA:641:U:C4'    | 1:AA:642:A:OP1     | 2.64                     | 0.45              |
| 1:AA:942:G:C2     | 1:AA:943:U:C2      | 3.04                     | 0.45              |
| 2:AB:144:ARG:O    | 2:AB:147:LYS:N     | 2.49                     | 0.45              |
| 2:AB:171:ALA:HA   | 2:AB:174:VAL:HG23  | 1.98                     | 0.45              |
| 4:AD:7:PRO:CB     | 4:AD:10:ARG:HD2    | 2.23                     | 0.45              |
| 4:AD:170:VAL:CG1  | 4:AD:174:LEU:HD12  | 2.46                     | 0.45              |
| 12:AL:34:CYS:HA   | 12:AL:55:VAL:HA    | 1.99                     | 0.45              |
| 13:AM:76:ALA:N    | 13:AM:79:LYS:NZ    | 2.60                     | 0.45              |
| 13:AM:93:ARG:HE   | 13:AM:93:ARG:CA    | 2.30                     | 0.45              |
| 20:AT:31:SER:O    | 20:AT:34:LYS:HB2   | 2.16                     | 0.45              |
| 23:AW:16:C:O2     | 23:AW:16:C:H3'     | 2.16                     | 0.45              |
| 51:B2:13:ALA:HA   | 51:B2:16:LEU:CD2   | 2.46                     | 0.45              |
| 27:BA:1346:G:C4   | 27:BA:1347:G:N7    | 2.84                     | 0.45              |
| 27:BA:140:G:H1'   | 27:BA:141:A:H2     | 1.79                     | 0.45              |
| 27:BA:1759:A:C5'  | 27:BA:2715:C:H1'   | 2.47                     | 0.45              |
| 27:BA:1835:G:C5   | 27:BA:1931:U:C4    | 3.04                     | 0.45              |
| 27:BA:2283:C:H2'  | 27:BA:2284:C:C5'   | 2.35                     | 0.45              |
| 27:BA:675:A:H2    | 27:BA:2443:C:O2    | 1.99                     | 0.45              |
| 27:BA:2512:C:H4'  | 31:BE:122:PHE:CE2  | 2.51                     | 0.45              |
| 27:BA:2642:G:C2   | 27:BA:2643:G:C4    | 3.04                     | 0.45              |
| 27:BA:335:C:C2    | 27:BA:336:C:C5     | 3.04                     | 0.45              |
| 27:BA:476:G:N2    | 27:BA:478:A:H3'    | 2.32                     | 0.45              |
| 27:BA:482:A:H8    | 27:BA:482:A:O5'    | 1.98                     | 0.45              |
| 27:BA:547:A:H8    | 27:BA:549:G:O6     | 1.99                     | 0.45              |
| 27:BA:563:G:H1    | 27:BA:578:A:H61    | 1.64                     | 0.45              |
| 27:BA:715:G:C2    | 27:BA:716:A:C4     | 3.04                     | 0.45              |
| 27:BA:748:G:OP1   | 27:BA:2612:C:N4    | 2.45                     | 0.45              |
| 27:BA:778:G:C2    | 27:BA:787:U:C2     | 3.04                     | 0.45              |
| 29:BC:181:PRO:O   | 29:BC:182:PRO:CB   | 2.64                     | 0.45              |
| 31:BE:39:PRO:HD3  | 31:BE:45:THR:OG1   | 2.17                     | 0.45              |
| 32:BF:8:GLN:HB3   | 32:BF:126:VAL:HA   | 1.98                     | 0.45              |
| 32:BF:83:PHE:O    | 32:BF:84:VAL:CB    | 2.44                     | 0.45              |
| 33:BG:11:TYR:CZ   | 33:BG:16:ARG:HG2   | 2.51                     | 0.45              |
| 33:BG:169:ALA:O   | 33:BG:172:LEU:HB3  | 2.15                     | 0.45              |
| 34:BH:101:ARG:CB  | 34:BH:117:PRO:HG3  | 2.44                     | 0.45              |
| 34:BH:149:ARG:HD3 | 34:BH:164:TYR:CE1  | 2.51                     | 0.45              |
| 35:BI:111:PRO:C   | 35:BI:114:LEU:HD11 | 2.37                     | 0.45              |
| 35:BI:5:LEU:CD1   | 35:BI:5:LEU:N      | 2.77                     | 0.45              |
| 37:BO:64:ARG:CZ   | 42:BT:70:VAL:HG21  | 2.46                     | 0.45              |
| 40:BR:116:LEU:HA  | 40:BR:116:LEU:HD23 | 1.77                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:BS:17:ARG:O    | 41:BS:18:ILE:CG2   | 2.64                     | 0.45              |
| 42:BT:20:PRO:O    | 42:BT:21:GLU:C     | 2.55                     | 0.45              |
| 45:BW:97:LYS:NZ   | 45:BW:99:ARG:HH12  | 2.15                     | 0.45              |
| 47:BY:26:LYS:CG   | 47:BY:27:VAL:H     | 2.04                     | 0.45              |
| 48:BZ:152:SER:OG  | 48:BZ:162:LEU:HD11 | 2.16                     | 0.45              |
| 48:BZ:25:GLY:O    | 48:BZ:26:VAL:HB    | 2.16                     | 0.45              |
| 1:CA:109:A:C8     | 1:CA:327:A:O4'     | 2.69                     | 0.45              |
| 1:CA:1270:C:O3'   | 1:CA:1314:C:H4'    | 2.15                     | 0.45              |
| 1:CA:176:C:H2'    | 1:CA:177:C:C6      | 2.49                     | 0.45              |
| 1:CA:51:A:C6      | 1:CA:353:A:C2      | 3.04                     | 0.45              |
| 1:CA:711:G:N2     | 1:CA:712:A:N3      | 2.64                     | 0.45              |
| 1:CA:833:U:H3     | 1:CA:853:G:H1      | 1.64                     | 0.45              |
| 1:CA:978:A:C5'    | 1:CA:978:A:H8      | 2.28                     | 0.45              |
| 2:CB:75:LYS:HD3   | 2:CB:78:GLN:HB2    | 1.97                     | 0.45              |
| 3:CC:186:PHE:CD1  | 3:CC:198:VAL:O     | 2.68                     | 0.45              |
| 4:CD:58:LEU:HD12  | 4:CD:59:ARG:NH1    | 2.31                     | 0.45              |
| 5:CE:101:ILE:N    | 5:CE:101:ILE:CD1   | 2.71                     | 0.45              |
| 5:CE:58:ALA:O     | 5:CE:61:TYR:HB2    | 2.15                     | 0.45              |
| 7:CG:143:ARG:HH11 | 7:CG:143:ARG:HB3   | 1.81                     | 0.45              |
| 7:CG:14:PRO:O     | 7:CG:15:ASP:O      | 2.34                     | 0.45              |
| 8:CH:128:GLY:O    | 8:CH:129:VAL:HG13  | 2.17                     | 0.45              |
| 1:CA:877:C:H1'    | 8:CH:3:THR:OG1     | 2.16                     | 0.45              |
| 10:CJ:54:PHE:CD1  | 10:CJ:55:LYS:HE3   | 2.52                     | 0.45              |
| 1:CA:963:G:N2     | 10:CJ:55:LYS:NZ    | 2.64                     | 0.45              |
| 1:CA:523:A:H61    | 12:CL:89:ASP:HB2   | 1.81                     | 0.45              |
| 14:CN:4:LYS:O     | 14:CN:8:GLU:HB2    | 2.15                     | 0.45              |
| 17:CQ:76:LEU:HD12 | 17:CQ:76:LEU:O     | 2.16                     | 0.45              |
| 17:CQ:80:GLY:O    | 17:CQ:81:ARG:HG2   | 2.15                     | 0.45              |
| 19:CS:39:THR:HG22 | 19:CS:40:ILE:O     | 2.16                     | 0.45              |
| 23:CW:74:C:H1'    | 27:DA:2507:C:O2'   | 2.16                     | 0.45              |
| 25:CY:3:G:H8      | 25:CY:3:G:O5'      | 1.99                     | 0.45              |
| 54:D5:56:LYS:H    | 54:D5:56:LYS:HD2   | 1.81                     | 0.45              |
| 27:DA:1409:C:H2'  | 27:DA:1410:G:C8    | 2.50                     | 0.45              |
| 27:DA:1411:C:O5'  | 27:DA:1411:C:C6    | 2.69                     | 0.45              |
| 27:DA:1558:A:O2'  | 27:DA:1559:G:OP2   | 2.30                     | 0.45              |
| 27:DA:1701:A:H2'  | 27:DA:1702:G:H5'   | 1.97                     | 0.45              |
| 27:DA:1763:G:H2'  | 27:DA:1764:G:H5'   | 1.98                     | 0.45              |
| 27:DA:1920:C:H2'  | 27:DA:1920:C:O2    | 2.16                     | 0.45              |
| 27:DA:1951:U:O2   | 27:DA:1953:A:H3'   | 2.15                     | 0.45              |
| 27:DA:2240:C:O2'  | 27:DA:2241:A:H5'   | 2.16                     | 0.45              |
| 27:DA:2638:G:P    | 31:DE:82:ARG:NH2   | 2.89                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2705:A:O5'   | 27:DA:2705:A:H8    | 1.99                     | 0.45              |
| 27:DA:867:C:H2'    | 27:DA:868:U:C5     | 2.50                     | 0.45              |
| 28:DB:68:C:O2'     | 28:DB:69:G:H5'     | 2.16                     | 0.45              |
| 28:DB:8:U:O2'      | 41:DS:40:ILE:HD13  | 2.16                     | 0.45              |
| 31:DE:16:ARG:HH11  | 31:DE:173:VAL:CG2  | 2.28                     | 0.45              |
| 32:DF:23:ASP:C     | 32:DF:24:LEU:HD22  | 2.35                     | 0.45              |
| 33:DG:111:LEU:HD21 | 33:DG:120:LEU:HD21 | 1.97                     | 0.45              |
| 33:DG:4:ASP:O      | 33:DG:4:ASP:OD1    | 2.34                     | 0.45              |
| 34:DH:157:TYR:O    | 34:DH:158:HIS:CB   | 2.64                     | 0.45              |
| 34:DH:19:VAL:HG13  | 34:DH:24:VAL:CG1   | 2.45                     | 0.45              |
| 34:DH:43:VAL:CG1   | 34:DH:53:GLU:H     | 2.30                     | 0.45              |
| 35:DI:4:ILE:O      | 35:DI:36:ALA:HB1   | 2.15                     | 0.45              |
| 37:DO:111:PHE:O    | 37:DO:112:MET:C    | 2.55                     | 0.45              |
| 37:DO:66:LYS:H     | 37:DO:82:ASN:HD21  | 1.63                     | 0.45              |
| 38:DP:21:ARG:O     | 38:DP:23:PRO:HD3   | 2.15                     | 0.45              |
| 46:DX:39:ILE:O     | 46:DX:40:LYS:C     | 2.54                     | 0.45              |
| 27:DA:481:G:O5'    | 47:DY:47:LYS:HE2   | 2.16                     | 0.45              |
| 48:DZ:54:HIS:CE1   | 48:DZ:134:GLU:HA   | 2.50                     | 0.45              |
| 48:DZ:60:LEU:CD2   | 48:DZ:60:LEU:H     | 2.29                     | 0.45              |
| 1:AA:1073:U:H2'    | 1:AA:1074:G:C8     | 2.49                     | 0.45              |
| 1:AA:1128:C:H1'    | 1:AA:1146:A:H61    | 1.81                     | 0.45              |
| 1:AA:1342:C:H2'    | 1:AA:1343:G:C8     | 2.51                     | 0.45              |
| 1:AA:1382:C:H2'    | 1:AA:1383:C:H6     | 1.81                     | 0.45              |
| 1:AA:966:G:O2'     | 1:AA:967:C:C5'     | 2.64                     | 0.45              |
| 2:AB:108:ILE:HD13  | 2:AB:108:ILE:HA    | 1.78                     | 0.45              |
| 2:AB:69:LEU:HB2    | 2:AB:159:PRO:HB3   | 1.98                     | 0.45              |
| 8:AH:53:VAL:O      | 8:AH:56:LYS:CG     | 2.63                     | 0.45              |
| 8:AH:76:PRO:O      | 8:AH:77:GLU:O      | 2.34                     | 0.45              |
| 12:AL:114:ARG:NH2  | 12:AL:121:LYS:CD   | 2.80                     | 0.45              |
| 15:AO:58:MET:O     | 15:AO:59:MET:C     | 2.54                     | 0.45              |
| 16:AP:1:MET:SD     | 16:AP:3:LYS:HG3    | 2.57                     | 0.45              |
| 20:AT:26:ASN:HB3   | 20:AT:71:THR:CG2   | 2.46                     | 0.45              |
| 24:AX:69:C:H2'     | 24:AX:70:G:O4'     | 2.16                     | 0.45              |
| 25:AY:57:A:C4'     | 25:AY:58:A:OP1     | 2.63                     | 0.45              |
| 49:B0:23:VAL:O     | 49:B0:24:LYS:HD3   | 2.16                     | 0.45              |
| 24:AX:1:C:O2       | 49:B0:5:LYS:HB3    | 2.15                     | 0.45              |
| 55:B6:25:LYS:HD2   | 55:B6:27:LYS:NZ    | 2.31                     | 0.45              |
| 55:B6:27:LYS:O     | 55:B6:28:ARG:C     | 2.54                     | 0.45              |
| 56:B7:17:GLY:O     | 56:B7:21:ARG:HG2   | 2.16                     | 0.45              |
| 57:B8:11:LYS:HE2   | 57:B8:64:TYR:HE1   | 1.81                     | 0.45              |
| 27:BA:1453:U:OP1   | 40:BR:77:ARG:NH1   | 2.45                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:1480:G:H2'   | 27:BA:1480:G:N3   | 2.32                     | 0.45              |
| 27:BA:1640:C:C2'   | 27:BA:1640:C:O2   | 2.60                     | 0.45              |
| 27:BA:174:C:O2     | 27:BA:174:C:H2'   | 2.15                     | 0.45              |
| 27:BA:2323:G:O2'   | 27:BA:2324:C:H5'  | 2.16                     | 0.45              |
| 27:BA:25:U:O5'     | 27:BA:25:U:H6     | 1.98                     | 0.45              |
| 27:BA:56:A:C2      | 27:BA:115:C:O2    | 2.69                     | 0.45              |
| 27:BA:766:C:C2     | 27:BA:767:U:C6    | 3.04                     | 0.45              |
| 27:BA:849:A:N6     | 27:BA:928:G:O2'   | 2.47                     | 0.45              |
| 28:BB:87:G:C2'     | 28:BB:88:C:H5''   | 2.46                     | 0.45              |
| 28:BB:95:C:O2'     | 28:BB:96:U:H5'    | 2.16                     | 0.45              |
| 29:BC:83:ILE:HD12  | 29:BC:94:VAL:HB   | 1.97                     | 0.45              |
| 31:BE:119:ARG:CD   | 31:BE:120:TRP:NE1 | 2.77                     | 0.45              |
| 32:BF:4:VAL:HA     | 32:BF:19:GLU:HB3  | 1.99                     | 0.45              |
| 32:BF:43:LYS:C     | 32:BF:45:ARG:H    | 2.19                     | 0.45              |
| 32:BF:89:VAL:CG1   | 32:BF:90:PHE:H    | 2.11                     | 0.45              |
| 33:BG:33:ARG:H     | 33:BG:162:THR:CG2 | 2.30                     | 0.45              |
| 33:BG:170:ARG:NH2  | 33:BG:182:LYS:HZ2 | 2.13                     | 0.45              |
| 37:BO:77:ILE:HD11  | 42:BT:72:VAL:HG12 | 1.96                     | 0.45              |
| 37:BO:91:LEU:N     | 37:BO:91:LEU:HD22 | 2.31                     | 0.45              |
| 48:BZ:124:LEU:HD23 | 48:BZ:163:ALA:O   | 2.16                     | 0.45              |
| 48:BZ:15:SER:HA    | 48:BZ:18:ARG:HD2  | 1.98                     | 0.45              |
| 1:CA:1067:A:H4'    | 1:CA:1068:G:O5'   | 2.16                     | 0.45              |
| 1:CA:1096:C:O2'    | 1:CA:1097:C:H5'   | 2.16                     | 0.45              |
| 1:CA:1298:C:H4'    | 1:CA:1299:A:C4    | 2.52                     | 0.45              |
| 1:CA:1319:A:H2'    | 1:CA:1323:G:N7    | 2.31                     | 0.45              |
| 1:CA:192:U:H4'     | 20:CT:103:GLY:CA  | 2.40                     | 0.45              |
| 1:CA:500:G:C2      | 1:CA:501:C:C2     | 3.04                     | 0.45              |
| 1:CA:662:G:O2'     | 1:CA:836:G:H5''   | 2.16                     | 0.45              |
| 2:CB:107:THR:O     | 2:CB:110:GLN:CG   | 2.64                     | 0.45              |
| 3:CC:147:LYS:CB    | 3:CC:203:PHE:CD2  | 3.00                     | 0.45              |
| 4:CD:49:ARG:O      | 4:CD:50:ARG:C     | 2.54                     | 0.45              |
| 4:CD:61:LYS:NZ     | 4:CD:62:GLN:HE21  | 2.12                     | 0.45              |
| 8:CH:6:ILE:CD1     | 8:CH:6:ILE:N      | 2.80                     | 0.45              |
| 8:CH:84:ARG:HH11   | 8:CH:84:ARG:HG2   | 1.82                     | 0.45              |
| 13:CM:81:LEU:HB3   | 13:CM:89:GLY:HA2  | 1.97                     | 0.45              |
| 1:CA:751:U:H1'     | 15:CO:24:SER:HA   | 1.98                     | 0.45              |
| 24:CX:10:G:H2'     | 24:CX:11:A:H8     | 1.80                     | 0.45              |
| 24:CX:25:C:O2'     | 24:CX:26:G:H5'    | 2.16                     | 0.45              |
| 50:D1:6:GLU:C      | 50:D1:7:ILE:HD12  | 2.36                     | 0.45              |
| 56:D7:24:THR:CG2   | 56:D7:27:GLY:H    | 2.26                     | 0.45              |
| 57:D8:4:MET:O      | 57:D8:62:LEU:CD1  | 2.57                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1341:U:C4    | 27:DA:1395:A:H2    | 2.34                     | 0.45              |
| 27:DA:1374:G:C2    | 27:DA:1375:C:C2    | 3.04                     | 0.45              |
| 27:DA:1497:U:C5'   | 27:DA:1498:C:C5    | 2.99                     | 0.45              |
| 27:DA:1693:U:C2'   | 30:DD:14:ARG:NH2   | 2.79                     | 0.45              |
| 27:DA:1770:G:C5    | 27:DA:1771:C:C5    | 3.05                     | 0.45              |
| 27:DA:1773:A:C2'   | 27:DA:1774:C:H5'   | 2.46                     | 0.45              |
| 27:DA:2016:U:C4    | 27:DA:2017:U:C4    | 3.04                     | 0.45              |
| 27:DA:2093:G:H2'   | 27:DA:2094:G:H8    | 1.81                     | 0.45              |
| 27:DA:2256:G:O2'   | 49:D0:9:SER:HB2    | 2.16                     | 0.45              |
| 27:DA:271(J):C:OP2 | 27:DA:271(J):C:H6  | 1.98                     | 0.45              |
| 27:DA:2749:A:O2'   | 34:DH:59:ARG:HG3   | 2.15                     | 0.45              |
| 27:DA:272(J):C:H3' | 27:DA:274:G:H21    | 1.81                     | 0.45              |
| 27:DA:405:U:O2'    | 27:DA:406:G:OP1    | 2.34                     | 0.45              |
| 27:DA:557:U:O5'    | 27:DA:557:U:H6     | 1.98                     | 0.45              |
| 27:DA:580:C:O3'    | 43:DU:31:SER:OG    | 2.32                     | 0.45              |
| 27:DA:612:C:C2'    | 27:DA:613:G:H5'    | 2.47                     | 0.45              |
| 27:DA:69:C:O2      | 27:DA:69:C:H2'     | 2.16                     | 0.45              |
| 27:DA:740:U:C4     | 27:DA:758:C:O2     | 2.70                     | 0.45              |
| 27:DA:783:A:H2'    | 27:DA:784:A:C5'    | 2.46                     | 0.45              |
| 27:DA:776:G:C4     | 27:DA:793:A:C2     | 3.04                     | 0.45              |
| 27:DA:566:U:H4'    | 27:DA:809:G:OP2    | 2.16                     | 0.45              |
| 27:DA:942:G:C6     | 27:DA:943:U:N3     | 2.84                     | 0.45              |
| 27:DA:955:C:O2'    | 27:DA:956:G:H5'    | 2.16                     | 0.45              |
| 27:DA:2126:A:H5'   | 29:DC:36:LYS:HG2   | 1.99                     | 0.45              |
| 30:DD:177:LEU:HB3  | 30:DD:178:PRO:HD2  | 1.98                     | 0.45              |
| 30:DD:27:THR:CG2   | 30:DD:27:THR:O     | 2.63                     | 0.45              |
| 31:DE:47:VAL:HG21  | 31:DE:85:ASN:HA    | 1.98                     | 0.45              |
| 32:DF:2:LYS:CD     | 32:DF:2:LYS:H      | 2.30                     | 0.45              |
| 34:DH:139:GLN:HG3  | 34:DH:140:LYS:N    | 2.32                     | 0.45              |
| 35:DI:76:THR:O     | 35:DI:77:LEU:O     | 2.33                     | 0.45              |
| 27:DA:1012:U:C4    | 36:DN:25:ARG:HD3   | 2.51                     | 0.45              |
| 36:DN:28:THR:HG23  | 36:DN:29:LYS:HG3   | 1.97                     | 0.45              |
| 39:DQ:10:ARG:O     | 39:DQ:10:ARG:CG    | 2.64                     | 0.45              |
| 44:DV:38:LEU:O     | 44:DV:39:LEU:HD13  | 2.15                     | 0.45              |
| 45:DW:24:ILE:HA    | 45:DW:27:LYS:HD2   | 1.97                     | 0.45              |
| 48:DZ:101:LEU:HB3  | 48:DZ:103:PHE:CE1  | 2.51                     | 0.45              |
| 48:DZ:143:LEU:N    | 48:DZ:143:LEU:HD22 | 2.31                     | 0.45              |
| 48:DZ:51:SER:OG    | 48:DZ:52:ILE:HD12  | 2.16                     | 0.45              |
| 48:DZ:55:VAL:HA    | 48:DZ:69:LEU:HD21  | 1.99                     | 0.45              |
| 1:AA:1444:C:O2'    | 1:AA:1445:C:H5'    | 2.17                     | 0.45              |
| 1:AA:781:A:O2'     | 1:AA:1522:U:O2     | 2.34                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:409:G:OP1    | 4:AD:25:ARG:N     | 2.43                     | 0.45              |
| 1:AA:559:A:O2'    | 1:AA:560:U:OP2    | 2.28                     | 0.45              |
| 1:AA:601:C:C2'    | 1:AA:602:A:H5'    | 2.45                     | 0.45              |
| 1:AA:997:U:H2'    | 1:AA:998:G:C8     | 2.51                     | 0.45              |
| 2:AB:83:MET:HA    | 2:AB:83:MET:HE2   | 1.97                     | 0.45              |
| 4:AD:100:ARG:CZ   | 4:AD:137:SER:HB3  | 2.46                     | 0.45              |
| 4:AD:57:ARG:HD3   | 4:AD:205:GLU:HB3  | 1.97                     | 0.45              |
| 1:AA:5:U:N3       | 4:AD:86:LYS:HE2   | 2.32                     | 0.45              |
| 8:AH:97:VAL:HG13  | 8:AH:98:LYS:HG3   | 1.98                     | 0.45              |
| 19:AS:6:LYS:CG    | 19:AS:7:LYS:HE3   | 2.46                     | 0.45              |
| 20:AT:48:LYS:O    | 20:AT:49:ALA:HB2  | 2.16                     | 0.45              |
| 23:AW:66:A:C5     | 23:AW:67:C:C4     | 3.05                     | 0.45              |
| 25:AY:37:U:H2'    | 25:AY:38:U:O4'    | 2.17                     | 0.45              |
| 49:B0:69:PHE:HD1  | 49:B0:69:PHE:N    | 2.14                     | 0.45              |
| 52:B3:31:LEU:O    | 52:B3:32:GLN:CB   | 2.65                     | 0.45              |
| 27:BA:1050:A:O2'  | 27:BA:1051:G:P    | 2.75                     | 0.45              |
| 27:BA:1204:A:HO2' | 27:BA:1205:U:P    | 2.36                     | 0.45              |
| 27:BA:1290:C:H2'  | 27:BA:1291:C:H6   | 1.82                     | 0.45              |
| 27:BA:1587:A:H3'  | 27:BA:1588:C:H6   | 1.81                     | 0.45              |
| 27:BA:1692:U:O2'  | 27:BA:1693:U:H2'  | 2.16                     | 0.45              |
| 27:BA:1899:G:N2   | 27:BA:1902:C:C5   | 2.85                     | 0.45              |
| 27:BA:2063:C:C5   | 27:BA:2064:C:C4   | 3.05                     | 0.45              |
| 27:BA:230:U:O5'   | 27:BA:230:U:H6    | 1.98                     | 0.45              |
| 27:BA:2735:G:H2'  | 27:BA:2736:G:H8   | 1.81                     | 0.45              |
| 27:BA:389:G:H1    | 38:BP:71:VAL:CG1  | 2.21                     | 0.45              |
| 27:BA:481:G:O2'   | 27:BA:482:A:OP2   | 2.22                     | 0.45              |
| 27:BA:533:G:C6    | 27:BA:561:G:N2    | 2.85                     | 0.45              |
| 27:BA:873:G:N1    | 27:BA:905:U:C2    | 2.85                     | 0.45              |
| 27:BA:958:U:O2'   | 27:BA:959:A:OP1   | 2.26                     | 0.45              |
| 27:BA:97:C:H5''   | 51:B2:2:LYS:HB3   | 1.99                     | 0.45              |
| 28:BB:45:A:C2     | 28:BB:46:A:C1'    | 2.99                     | 0.45              |
| 29:BC:22:ILE:CG2  | 29:BC:24:GLU:HB2  | 2.46                     | 0.45              |
| 29:BC:78:ALA:HB2  | 29:BC:82:LYS:HD2  | 1.98                     | 0.45              |
| 30:BD:53:PHE:O    | 30:BD:218:ARG:HG3 | 2.15                     | 0.45              |
| 30:BD:34:VAL:O    | 30:BD:34:VAL:CG1  | 2.57                     | 0.45              |
| 30:BD:48:ARG:HG2  | 30:BD:48:ARG:H    | 1.33                     | 0.45              |
| 30:BD:58:HIS:CD2  | 30:BD:59:LYS:N    | 2.84                     | 0.45              |
| 30:BD:65:ILE:HG12 | 30:BD:104:TYR:C   | 2.36                     | 0.45              |
| 32:BF:172:TRP:N   | 32:BF:172:TRP:CD1 | 2.85                     | 0.45              |
| 33:BG:51:ARG:HE   | 33:BG:51:ARG:HA   | 1.78                     | 0.45              |
| 34:BH:158:HIS:ND1 | 34:BH:168:PRO:HB2 | 2.30                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BH:71:LEU:H    | 34:BH:74:ASN:HD22 | 1.64                     | 0.45              |
| 37:BO:35:VAL:HG21 | 37:BO:69:ILE:HD13 | 1.99                     | 0.45              |
| 27:BA:625:G:O6    | 38:BP:107:LYS:HD2 | 2.16                     | 0.45              |
| 38:BP:97:PRO:C    | 38:BP:99:LEU:N    | 2.70                     | 0.45              |
| 40:BR:71:GLN:HE21 | 40:BR:71:GLN:HB2  | 1.57                     | 0.45              |
| 41:BS:85:VAL:CG2  | 41:BS:106:ARG:HB2 | 2.45                     | 0.45              |
| 42:BT:134:GLU:O   | 42:BT:135:ALA:CB  | 2.62                     | 0.45              |
| 43:BU:66:ASN:HB2  | 43:BU:76:TYR:HB2  | 1.99                     | 0.45              |
| 39:BQ:25:ASP:O    | 48:BZ:80:ARG:NH2  | 2.48                     | 0.45              |
| 1:CA:123:C:H5''   | 1:CA:311:C:O2'    | 2.17                     | 0.45              |
| 1:CA:1286:A:H2'   | 1:CA:1287:A:H4'   | 1.98                     | 0.45              |
| 1:CA:1494:G:N2    | 1:CA:1495:U:C2    | 2.85                     | 0.45              |
| 1:CA:266:G:H1     | 1:CA:271:C:H42    | 1.64                     | 0.45              |
| 1:CA:508:C:C4'    | 1:CA:509:A:OP1    | 2.60                     | 0.45              |
| 1:CA:583:A:H8     | 1:CA:583:A:O5'    | 1.99                     | 0.45              |
| 1:CA:59:A:C5'     | 1:CA:60:A:C5'     | 2.94                     | 0.45              |
| 1:CA:638:G:O2'    | 1:CA:639:G:H5'    | 2.17                     | 0.45              |
| 1:CA:789:U:O2     | 1:CA:792:A:C8     | 2.69                     | 0.45              |
| 1:CA:913:A:C1'    | 1:CA:914:A:O4'    | 2.65                     | 0.45              |
| 2:CB:43:ASP:OD2   | 2:CB:46:LYS:N     | 2.49                     | 0.45              |
| 3:CC:196:LEU:HD12 | 3:CC:197:GLY:N    | 2.32                     | 0.45              |
| 3:CC:36:ASP:OD2   | 3:CC:57:ILE:HG21  | 2.16                     | 0.45              |
| 4:CD:138:TYR:C    | 4:CD:138:TYR:HD2  | 2.20                     | 0.45              |
| 5:CE:40:ARG:HB3   | 5:CE:66:MET:HE1   | 1.95                     | 0.45              |
| 6:CF:23:LYS:HB3   | 6:CF:23:LYS:HE2   | 1.78                     | 0.45              |
| 6:CF:32:ASN:C     | 6:CF:34:GLY:N     | 2.69                     | 0.45              |
| 7:CG:79:ARG:HA    | 7:CG:84:ASN:HA    | 1.98                     | 0.45              |
| 9:CI:18:PHE:CD1   | 9:CI:62:TYR:HD2   | 2.35                     | 0.45              |
| 9:CI:17:VAL:HG11  | 9:CI:81:ILE:HD13  | 1.98                     | 0.45              |
| 12:CL:66:TYR:HB2  | 12:CL:93:VAL:HG11 | 1.98                     | 0.45              |
| 13:CM:99:ARG:HB2  | 13:CM:101:GLN:NE2 | 2.31                     | 0.45              |
| 1:CA:237:C:C5'    | 17:CQ:25:ARG:NH1  | 2.77                     | 0.45              |
| 18:CR:50:ILE:CD1  | 18:CR:70:ILE:HG21 | 2.45                     | 0.45              |
| 20:CT:18:GLN:O    | 20:CT:19:SER:C    | 2.54                     | 0.45              |
| 51:D2:56:GLN:O    | 51:D2:57:ILE:C    | 2.55                     | 0.45              |
| 55:D6:32:ASN:ND2  | 55:D6:33:LYS:N    | 2.44                     | 0.45              |
| 55:D6:34:LEU:O    | 55:D6:36:LEU:HG   | 2.16                     | 0.45              |
| 27:DA:1292:U:H2'  | 27:DA:1293:C:H6   | 1.79                     | 0.45              |
| 27:DA:1275:A:H2   | 27:DA:1295:C:O2   | 1.99                     | 0.45              |
| 27:DA:1478:G:N2   | 27:DA:1558:A:OP1  | 2.50                     | 0.45              |
| 27:DA:1599:C:OP1  | 46:DX:35:THR:HA   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:1862:G:H1   | 27:DA:1880:C:N4    | 2.04                     | 0.45              |
| 27:DA:1845:G:C4   | 27:DA:1896:G:C2    | 3.04                     | 0.45              |
| 27:DA:2308:G:N2   | 27:DA:2309:A:N1    | 2.65                     | 0.45              |
| 27:DA:2420:C:OP1  | 57:D8:34:TRP:HA    | 2.16                     | 0.45              |
| 27:DA:2642:G:H2'  | 27:DA:2643:G:O4'   | 2.15                     | 0.45              |
| 27:DA:2702:U:O2   | 27:DA:2702:U:C2'   | 2.63                     | 0.45              |
| 27:DA:2715:C:H2'  | 27:DA:2716:U:H6    | 1.81                     | 0.45              |
| 27:DA:2746:U:O5'  | 27:DA:2746:U:H6    | 2.00                     | 0.45              |
| 27:DA:573:G:O6    | 27:DA:2029:G:H2'   | 2.17                     | 0.45              |
| 27:DA:691:C:O2'   | 27:DA:692:C:H5'    | 2.15                     | 0.45              |
| 27:DA:736:C:HO2'  | 27:DA:737:C:H5'    | 1.81                     | 0.45              |
| 27:DA:815:C:H2'   | 27:DA:816:C:C6     | 2.52                     | 0.45              |
| 27:DA:839:U:H2'   | 27:DA:840:C:C5     | 2.52                     | 0.45              |
| 29:DC:18:LYS:CD   | 29:DC:19:VAL:H     | 2.27                     | 0.45              |
| 29:DC:41:VAL:CA   | 29:DC:213:TYR:HA   | 2.46                     | 0.45              |
| 33:DG:7:LEU:HA    | 33:DG:7:LEU:HD23   | 1.67                     | 0.45              |
| 35:DI:30:LEU:O    | 35:DI:31:LEU:C     | 2.55                     | 0.45              |
| 36:DN:57:ALA:O    | 36:DN:58:ASP:O     | 2.34                     | 0.45              |
| 37:DO:13:ASN:O    | 37:DO:15:GLY:N     | 2.49                     | 0.45              |
| 38:DP:125:VAL:O   | 38:DP:125:VAL:CG2  | 2.64                     | 0.45              |
| 27:DA:832:G:N3    | 38:DP:53:GLY:HA2   | 2.32                     | 0.45              |
| 43:DU:76:TYR:OH   | 43:DU:93:LYS:HE3   | 2.17                     | 0.45              |
| 44:DV:71:LEU:HD13 | 44:DV:84:LYS:HE2   | 1.97                     | 0.45              |
| 45:DW:54:ALA:HB1  | 45:DW:107:LEU:HD13 | 1.99                     | 0.45              |
| 48:DZ:126:LYS:O   | 48:DZ:126:LYS:HG2  | 2.17                     | 0.45              |
| 48:DZ:69:LEU:HD23 | 48:DZ:69:LEU:HA    | 1.79                     | 0.45              |
| 1:AA:1156:G:O5'   | 1:AA:1156:G:H8     | 1.99                     | 0.45              |
| 1:AA:1264:C:H6    | 1:AA:1264:C:H3'    | 1.79                     | 0.45              |
| 1:AA:1270:C:C2'   | 1:AA:1271:G:H5'    | 2.46                     | 0.45              |
| 1:AA:1306:A:H2'   | 1:AA:1307:U:C6     | 2.51                     | 0.45              |
| 1:AA:946:A:O2'    | 1:AA:1333:A:N3     | 2.28                     | 0.45              |
| 1:AA:1339:A:N6    | 1:AA:1340:A:N3     | 2.64                     | 0.45              |
| 1:AA:1511:G:H2'   | 1:AA:1512:U:O4'    | 2.17                     | 0.45              |
| 1:AA:109:A:C8     | 1:AA:326:G:H2'     | 2.51                     | 0.45              |
| 1:AA:318:G:H1     | 1:AA:335:C:H42     | 1.64                     | 0.45              |
| 1:AA:504:C:C2     | 1:AA:542:G:N2      | 2.85                     | 0.45              |
| 1:AA:775:G:O2'    | 1:AA:776:G:H5'     | 2.17                     | 0.45              |
| 1:AA:939:G:P      | 7:AG:102:ARG:HH12  | 2.40                     | 0.45              |
| 2:AB:76:GLN:O     | 2:AB:208:ILE:HG12  | 2.17                     | 0.45              |
| 2:AB:77:ALA:HB2   | 2:AB:211:ILE:CD1   | 2.47                     | 0.45              |
| 1:AA:401:C:OP2    | 4:AD:73:ARG:NH2    | 2.50                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:AF:61:LEU:HD23   | 6:AF:63:TYR:HE2     | 1.81                     | 0.45              |
| 6:AF:74:ASP:O      | 6:AF:77:ARG:HB3     | 2.17                     | 0.45              |
| 7:AG:4:ARG:HD3     | 7:AG:5:ARG:NH1      | 2.31                     | 0.45              |
| 8:AH:104:ARG:NH2   | 8:AH:138:TRP:CH2    | 2.84                     | 0.45              |
| 9:AI:50:LEU:O      | 9:AI:54:ASP:N       | 2.50                     | 0.45              |
| 10:AJ:32:ALA:CB    | 10:AJ:76:ASN:HB2    | 2.46                     | 0.45              |
| 10:AJ:7:LYS:HB2    | 10:AJ:97:GLU:HB2    | 1.99                     | 0.45              |
| 12:AL:110:ARG:HH11 | 12:AL:110:ARG:HG2   | 1.81                     | 0.45              |
| 12:AL:73:ASN:O     | 12:AL:74:LEU:O      | 2.34                     | 0.45              |
| 16:AP:8:ARG:NH2    | 16:AP:15:PRO:HG3    | 2.32                     | 0.45              |
| 17:AQ:26:GLN:HB3   | 17:AQ:37:LYS:CG     | 2.39                     | 0.45              |
| 17:AQ:27:PHE:HB2   | 17:AQ:28:PRO:CD     | 2.46                     | 0.45              |
| 18:AR:45:SER:OG    | 18:AR:49:LYS:N      | 2.49                     | 0.45              |
| 18:AR:63:GLN:O     | 18:AR:66:LEU:HB3    | 2.16                     | 0.45              |
| 19:AS:31:ILE:O     | 19:AS:31:ILE:HG23   | 2.16                     | 0.45              |
| 23:AW:64:G:H5'     | 23:AW:65:U:OP2      | 2.17                     | 0.45              |
| 57:B8:11:LYS:H     | 57:B8:60:LEU:HD21   | 1.82                     | 0.45              |
| 58:B9:27:CYS:HB2   | 58:B9:32:HIS:HB2    | 1.97                     | 0.45              |
| 58:B9:27:CYS:SG    | 58:B9:32:HIS:HB2    | 2.57                     | 0.45              |
| 27:BA:1331:A:H2'   | 27:BA:1333:C:H5     | 1.82                     | 0.45              |
| 27:BA:142:A:H1'    | 27:BA:1408:C:H1'    | 1.98                     | 0.45              |
| 27:BA:1450:G:H2'   | 27:BA:1450(A):C:H5' | 1.99                     | 0.45              |
| 27:BA:182:A:H2'    | 27:BA:183:C:C6      | 2.52                     | 0.45              |
| 27:BA:1838:C:O2'   | 27:BA:1898:U:C5     | 2.69                     | 0.45              |
| 27:BA:1992:G:C6    | 27:BA:1997:G:N1     | 2.84                     | 0.45              |
| 27:BA:2082:A:H2'   | 27:BA:2083:G:H8     | 1.80                     | 0.45              |
| 27:BA:2291:U:OP1   | 27:BA:2381:C:H5'    | 2.17                     | 0.45              |
| 27:BA:2482:G:H2'   | 27:BA:2483:C:C6     | 2.49                     | 0.45              |
| 27:BA:2737:G:H2'   | 27:BA:2738:A:C8     | 2.52                     | 0.45              |
| 27:BA:2745:C:H42   | 27:BA:2759:G:H1     | 1.63                     | 0.45              |
| 27:BA:391:G:C6     | 27:BA:392:C:C4      | 3.04                     | 0.45              |
| 27:BA:23:G:H1      | 27:BA:517:C:H42     | 1.63                     | 0.45              |
| 27:BA:576:U:H2'    | 27:BA:577:G:H8      | 1.75                     | 0.45              |
| 27:BA:642:G:N1     | 27:BA:645:C:OP2     | 2.50                     | 0.45              |
| 27:BA:711:G:C2     | 27:BA:721:C:C2      | 3.04                     | 0.45              |
| 27:BA:92:A:O2'     | 27:BA:93:G:OP2      | 2.26                     | 0.45              |
| 27:BA:975(A):G:O2' | 27:BA:976:C:H5'     | 2.16                     | 0.45              |
| 30:BD:138:VAL:HG23 | 30:BD:165:ILE:HG22  | 1.98                     | 0.45              |
| 30:BD:232:PRO:HD2  | 30:BD:249:PRO:HA    | 1.97                     | 0.45              |
| 31:BE:36:ARG:HG2   | 31:BE:36:ARG:NH1    | 2.32                     | 0.45              |
| 27:BA:607:U:OP1    | 32:BF:103:LYS:HG3   | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:BF:3:GLU:C     | 32:BF:19:GLU:HB3  | 2.37                     | 0.45              |
| 32:BF:67:GLN:O    | 32:BF:68:LYS:CB   | 2.54                     | 0.45              |
| 37:BO:87:ILE:HG23 | 37:BO:92:GLU:O    | 2.16                     | 0.45              |
| 32:BF:34:TRP:CE2  | 38:BP:12:ALA:HB2  | 2.51                     | 0.45              |
| 38:BP:75:ILE:N    | 38:BP:75:ILE:HD12 | 2.32                     | 0.45              |
| 40:BR:4:LEU:O     | 40:BR:6:SER:N     | 2.49                     | 0.45              |
| 41:BS:17:ARG:CA   | 41:BS:20:ARG:NH1  | 2.79                     | 0.45              |
| 41:BS:66:ALA:O    | 41:BS:67:ARG:C    | 2.55                     | 0.45              |
| 42:BT:19:LEU:HA   | 42:BT:20:PRO:HD3  | 1.78                     | 0.45              |
| 46:BX:35:THR:OG1  | 46:BX:38:GLU:HB2  | 2.16                     | 0.45              |
| 47:BY:5:MET:HA    | 47:BY:5:MET:CE    | 2.47                     | 0.45              |
| 48:BZ:131:ASN:ND2 | 48:BZ:131:ASN:N   | 2.64                     | 0.45              |
| 48:BZ:33:ASN:O    | 48:BZ:33:ASN:OD1  | 2.34                     | 0.45              |
| 1:CA:1198:G:C2    | 1:CA:1199:U:C2    | 3.05                     | 0.45              |
| 1:CA:1232:U:C2'   | 1:CA:1233:G:O5'   | 2.64                     | 0.45              |
| 1:CA:1239:A:H5'   | 1:CA:1240:U:OP1   | 2.17                     | 0.45              |
| 1:CA:1255:G:O2'   | 1:CA:1258:G:H1'   | 2.15                     | 0.45              |
| 1:CA:978:A:H1'    | 1:CA:1322:C:O2    | 2.16                     | 0.45              |
| 1:CA:1311:G:N2    | 1:CA:1327:C:C2    | 2.84                     | 0.45              |
| 1:CA:1499:A:C2    | 1:CA:1500:A:C8    | 3.05                     | 0.45              |
| 1:CA:266:G:H5''   | 1:CA:267:C:C5     | 2.51                     | 0.45              |
| 1:CA:336:C:O2'    | 1:CA:337:C:H5'    | 2.16                     | 0.45              |
| 1:CA:39:G:O2'     | 1:CA:40:C:H5'     | 2.16                     | 0.45              |
| 1:CA:514:C:O2'    | 1:CA:515:G:H5'    | 2.16                     | 0.45              |
| 1:CA:707:C:O2     | 11:CK:39:PRO:HD3  | 2.16                     | 0.45              |
| 1:CA:735:C:O2'    | 1:CA:736:C:H5'    | 2.16                     | 0.45              |
| 1:CA:818:G:N3     | 1:CA:820:U:C6     | 2.84                     | 0.45              |
| 2:CB:140:HIS:O    | 2:CB:143:GLU:HB2  | 2.16                     | 0.45              |
| 2:CB:213:LEU:O    | 2:CB:213:LEU:HD23 | 2.16                     | 0.45              |
| 2:CB:91:PRO:HG2   | 2:CB:155:LEU:HD23 | 1.98                     | 0.45              |
| 4:CD:182:LYS:HB2  | 4:CD:183:GLY:H    | 1.41                     | 0.45              |
| 5:CE:87:SER:CB    | 5:CE:131:ILE:HD13 | 2.47                     | 0.45              |
| 5:CE:31:LEU:HD11  | 5:CE:43:LEU:HD21  | 1.97                     | 0.45              |
| 4:CD:88:VAL:HG13  | 5:CE:97:GLY:HA3   | 1.98                     | 0.45              |
| 7:CG:32:ARG:O     | 7:CG:33:ASP:CB    | 2.65                     | 0.45              |
| 10:CJ:87:THR:O    | 10:CJ:88:LEU:C    | 2.54                     | 0.45              |
| 13:CM:91:ARG:O    | 13:CM:96:LEU:O    | 2.34                     | 0.45              |
| 57:D8:63:PRO:HB2  | 57:D8:64:TYR:CD1  | 2.51                     | 0.45              |
| 27:DA:1187:G:C8   | 27:DA:1187:G:O5'  | 2.56                     | 0.45              |
| 27:DA:1216:G:N3   | 27:DA:1216:G:H2'  | 2.32                     | 0.45              |
| 27:DA:1321:A:H2'  | 27:DA:1322:A:H8   | 1.80                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1746:G:N3    | 27:DA:1746:G:H2'   | 2.31                     | 0.45              |
| 27:DA:205:G:O2'    | 27:DA:206:U:P      | 2.74                     | 0.45              |
| 27:DA:2242:G:H2'   | 27:DA:2243:U:O4'   | 2.17                     | 0.45              |
| 27:DA:2363:C:O2'   | 27:DA:2364:C:H5'   | 2.16                     | 0.45              |
| 27:DA:2392:A:H2'   | 27:DA:2393:A:O4'   | 2.16                     | 0.45              |
| 27:DA:2649:U:O2'   | 27:DA:2650:U:H5'   | 2.17                     | 0.45              |
| 27:DA:271(Q):G:OP1 | 35:DI:42:SER:HB2   | 2.17                     | 0.45              |
| 27:DA:271(W):G:C5' | 27:DA:271(X):G:OP2 | 2.64                     | 0.45              |
| 27:DA:555:U:C2'    | 27:DA:556:G:C8     | 3.00                     | 0.45              |
| 27:DA:614(C):A:C4' | 27:DA:615:G:OP1    | 2.64                     | 0.45              |
| 27:DA:700:G:H2'    | 27:DA:701:G:C8     | 2.51                     | 0.45              |
| 27:DA:8:A:H2'      | 27:DA:9:U:H6       | 1.73                     | 0.45              |
| 29:DC:59:ARG:CD    | 29:DC:59:ARG:N     | 2.78                     | 0.45              |
| 30:DD:117:VAL:HG23 | 30:DD:118:VAL:N    | 2.31                     | 0.45              |
| 30:DD:172:TYR:HD1  | 30:DD:186:HIS:N    | 2.15                     | 0.45              |
| 33:DG:22:ARG:HH11  | 33:DG:22:ARG:CB    | 2.08                     | 0.45              |
| 35:DI:51:ILE:CG2   | 35:DI:52:ARG:N     | 2.79                     | 0.45              |
| 37:DO:101:PRO:HD2  | 42:DT:70:VAL:HG21  | 1.95                     | 0.45              |
| 38:DP:21:ARG:HG2   | 38:DP:29:LYS:HE3   | 1.99                     | 0.45              |
| 39:DQ:32:TYR:O     | 39:DQ:106:VAL:HG22 | 2.17                     | 0.45              |
| 41:DS:67:ARG:CG    | 41:DS:67:ARG:NH1   | 2.77                     | 0.45              |
| 42:DT:96:ARG:HG3   | 42:DT:99:LEU:HB3   | 1.99                     | 0.45              |
| 44:DV:18:LEU:N     | 44:DV:18:LEU:CD1   | 2.79                     | 0.45              |
| 46:DX:57:LEU:CD1   | 46:DX:78:LYS:HD3   | 2.43                     | 0.45              |
| 46:DX:88:LYS:HE3   | 46:DX:90:GLU:OE2   | 2.16                     | 0.45              |
| 48:DZ:43:PHE:HE2   | 48:DZ:87:PHE:CZ    | 2.34                     | 0.45              |
| 1:AA:106:C:H2'     | 1:AA:107:G:H8      | 1.82                     | 0.45              |
| 1:AA:1112:C:O2     | 3:AC:179:ARG:HG2   | 2.16                     | 0.45              |
| 1:AA:1131:G:C2     | 1:AA:1132:C:N4     | 2.85                     | 0.45              |
| 1:AA:336:C:H1'     | 1:AA:1468:A:C2     | 2.52                     | 0.45              |
| 1:AA:203:U:H4'     | 1:AA:204:U:OP1     | 2.17                     | 0.45              |
| 1:AA:225:C:H2'     | 1:AA:226:G:C8      | 2.51                     | 0.45              |
| 1:AA:262:A:H5'     | 20:AT:74:LYS:HB2   | 1.97                     | 0.45              |
| 1:AA:413:G:H1'     | 1:AA:428:G:N2      | 2.31                     | 0.45              |
| 1:AA:428:G:HO2'    | 1:AA:429:U:P       | 2.39                     | 0.45              |
| 1:AA:636:U:H2'     | 1:AA:637:G:H8      | 1.82                     | 0.45              |
| 1:AA:797:C:H2'     | 1:AA:798:G:H8      | 1.81                     | 0.45              |
| 1:AA:823:G:C2'     | 1:AA:824:C:H5'     | 2.46                     | 0.45              |
| 2:AB:137:ARG:CD    | 2:AB:137:ARG:C     | 2.84                     | 0.45              |
| 3:AC:58:GLU:O      | 3:AC:59:ARG:HG2    | 2.17                     | 0.45              |
| 4:AD:127:THR:HA    | 4:AD:132:ARG:HA    | 1.98                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AD:13:ARG:C     | 4:AD:15:GLU:H      | 2.19                     | 0.45              |
| 4:AD:33:MET:HE1   | 4:AD:37:PRO:HA     | 1.93                     | 0.45              |
| 16:AP:48:TRP:O    | 16:AP:48:TRP:HE3   | 1.99                     | 0.45              |
| 17:AQ:67:LYS:CA   | 17:AQ:70:ARG:HH12  | 2.30                     | 0.45              |
| 50:B1:3:LYS:C     | 50:B1:4:VAL:HG12   | 2.37                     | 0.45              |
| 50:B1:86:SER:O    | 50:B1:87:PRO:C     | 2.52                     | 0.45              |
| 55:B6:41:PRO:CD   | 55:B6:46:HIS:N     | 2.80                     | 0.45              |
| 57:B8:7:HIS:CB    | 57:B8:59:LYS:HB3   | 2.46                     | 0.45              |
| 27:BA:2742:C:P    | 58:B9:35:ARG:HH11  | 2.40                     | 0.45              |
| 27:BA:1167:U:H2'  | 27:BA:1168:G:C8    | 2.51                     | 0.45              |
| 27:BA:1722:A:O2'  | 27:BA:1739:U:C5'   | 2.60                     | 0.45              |
| 27:BA:528:A:C2    | 27:BA:2042:A:H2'   | 2.52                     | 0.45              |
| 27:BA:2267:A:C2'  | 27:BA:2267:A:N3    | 2.77                     | 0.45              |
| 27:BA:858:U:O2'   | 27:BA:2268:A:H1'   | 2.16                     | 0.45              |
| 27:BA:2552:U:C2   | 27:BA:2554:U:H5'   | 2.50                     | 0.45              |
| 27:BA:2643:G:H1   | 27:BA:2771:C:H42   | 1.65                     | 0.45              |
| 27:BA:2706:G:H2'  | 27:BA:2707:G:O4'   | 2.17                     | 0.45              |
| 27:BA:2722:G:H2'  | 27:BA:2723:C:C6    | 2.51                     | 0.45              |
| 27:BA:2846:G:H2'  | 27:BA:2847:U:C6    | 2.52                     | 0.45              |
| 27:BA:2852:G:P    | 40:BR:64:ARG:HH22  | 2.40                     | 0.45              |
| 27:BA:2888:C:H2'  | 27:BA:2889:C:O4'   | 2.17                     | 0.45              |
| 27:BA:247:G:H4'   | 27:BA:386:G:C6     | 2.50                     | 0.45              |
| 27:BA:705:A:C6    | 27:BA:706:A:C5     | 3.04                     | 0.45              |
| 30:BD:12:SER:O    | 30:BD:14:ARG:N     | 2.50                     | 0.45              |
| 30:BD:69:ARG:NH2  | 30:BD:192:THR:HB   | 2.32                     | 0.45              |
| 31:BE:170:LEU:HB3 | 31:BE:184:VAL:HG13 | 1.99                     | 0.45              |
| 27:BA:2059:A:O2'  | 32:BF:69:HIS:HD2   | 1.99                     | 0.45              |
| 33:BG:97:ASP:O    | 33:BG:100:TRP:N    | 2.49                     | 0.45              |
| 34:BH:138:LYS:O   | 34:BH:142:GLY:N    | 2.47                     | 0.45              |
| 34:BH:64:LEU:O    | 34:BH:65:HIS:C     | 2.53                     | 0.45              |
| 35:BI:27:ARG:HD2  | 50:B1:71:TYR:CE1   | 2.52                     | 0.45              |
| 35:BI:52:ARG:HA   | 35:BI:55:ALA:HB3   | 1.99                     | 0.45              |
| 36:BN:62:VAL:HG22 | 36:BN:66:LYS:HB2   | 1.92                     | 0.45              |
| 36:BN:94:HIS:N    | 36:BN:95:PRO:HD2   | 2.32                     | 0.45              |
| 27:BA:2392:A:H1'  | 38:BP:60:MET:HB3   | 1.99                     | 0.45              |
| 42:BT:123:GLN:HG3 | 42:BT:123:GLN:O    | 2.15                     | 0.45              |
| 43:BU:114:LYS:O   | 43:BU:117:GLN:O    | 2.35                     | 0.45              |
| 44:BV:99:ILE:CG1  | 44:BV:99:ILE:O     | 2.58                     | 0.45              |
| 46:BX:14:SER:C    | 46:BX:16:LYS:N     | 2.67                     | 0.45              |
| 46:BX:12:VAL:HG12 | 46:BX:27:THR:HG23  | 1.98                     | 0.45              |
| 47:BY:32:PRO:HB2  | 47:BY:35:TYR:HA    | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1010:G:N2    | 1:CA:1020:U:H1'   | 2.32                     | 0.45              |
| 1:CA:1028:C:H2'   | 1:CA:1033:G:H22   | 1.81                     | 0.45              |
| 1:CA:1110:A:H8    | 1:CA:1110:A:O5'   | 1.99                     | 0.45              |
| 1:CA:1120:G:O2'   | 1:CA:1121:U:H5'   | 2.17                     | 0.45              |
| 1:CA:1228:C:H2'   | 1:CA:1229:A:H8    | 1.82                     | 0.45              |
| 1:CA:486:U:C2'    | 1:CA:487:A:H8     | 2.29                     | 0.45              |
| 1:CA:498:U:O2'    | 1:CA:499:A:P      | 2.75                     | 0.45              |
| 1:CA:542:G:O2'    | 1:CA:543:C:H5'    | 2.15                     | 0.45              |
| 1:CA:606:G:H2'    | 1:CA:631:G:H22    | 1.81                     | 0.45              |
| 1:CA:634:C:H2'    | 1:CA:635:G:H8     | 1.82                     | 0.45              |
| 1:CA:66:G:N2      | 1:CA:67:C:C1'     | 2.80                     | 0.45              |
| 1:CA:683:G:C6     | 1:CA:684:A:C6     | 3.05                     | 0.45              |
| 1:CA:725:G:O2'    | 1:CA:726:C:H5'    | 2.17                     | 0.45              |
| 1:CA:865:A:C6     | 1:CA:866:C:N3     | 2.85                     | 0.45              |
| 2:CB:91:PRO:HG2   | 2:CB:155:LEU:HG   | 1.99                     | 0.45              |
| 4:CD:153:ARG:CB   | 4:CD:153:ARG:HH11 | 2.14                     | 0.45              |
| 6:CF:43:LEU:HD12  | 6:CF:43:LEU:N     | 2.29                     | 0.45              |
| 6:CF:67:MET:HB2   | 6:CF:68:PRO:HD2   | 1.99                     | 0.45              |
| 6:CF:69:GLU:H     | 6:CF:69:GLU:CD    | 2.20                     | 0.45              |
| 6:CF:72:VAL:O     | 6:CF:72:VAL:CG2   | 2.65                     | 0.45              |
| 1:CA:1240:U:O3'   | 7:CG:38:LEU:HD21  | 2.16                     | 0.45              |
| 7:CG:67:GLU:O     | 7:CG:70:LYS:HB2   | 2.16                     | 0.45              |
| 8:CH:6:ILE:O      | 8:CH:7:ALA:C      | 2.54                     | 0.45              |
| 9:CI:64:THR:O     | 9:CI:64:THR:HG23  | 2.16                     | 0.45              |
| 10:CJ:22:LYS:CE   | 10:CJ:23:ILE:HG12 | 2.46                     | 0.45              |
| 1:CA:538:G:OP1    | 12:CL:110:ARG:HD2 | 2.17                     | 0.45              |
| 12:CL:48:ALA:O    | 12:CL:49:LEU:HD22 | 2.17                     | 0.45              |
| 14:CN:44:LEU:C    | 14:CN:44:LEU:HD12 | 2.36                     | 0.45              |
| 16:CP:12:LYS:HD3  | 16:CP:13:HIS:CD2  | 2.52                     | 0.45              |
| 16:CP:57:ARG:NH1  | 16:CP:79:VAL:O    | 2.49                     | 0.45              |
| 17:CQ:76:LEU:HD12 | 17:CQ:78:GLU:H    | 1.81                     | 0.45              |
| 20:CT:62:LEU:O    | 20:CT:65:LYS:HB2  | 2.16                     | 0.45              |
| 22:CV:7:C:H2'     | 22:CV:8:A:C8      | 2.49                     | 0.45              |
| 23:CW:20:A:N6     | 23:CW:44:A:C2'    | 2.79                     | 0.45              |
| 50:D1:70:VAL:O    | 50:D1:73:LEU:N    | 2.49                     | 0.45              |
| 51:D2:38:GLN:O    | 51:D2:45:SER:HB2  | 2.17                     | 0.45              |
| 51:D2:4:SER:OG    | 51:D2:7:ARG:HD2   | 2.16                     | 0.45              |
| 52:D3:8:LEU:HD13  | 52:D3:31:LEU:HD23 | 1.98                     | 0.45              |
| 27:DA:1286:A:O2'  | 27:DA:1288:U:OP2  | 2.19                     | 0.45              |
| 27:DA:1418:G:H8   | 27:DA:1418:G:O5'  | 2.00                     | 0.45              |
| 27:DA:1560:G:C2   | 27:DA:1561:G:H1'  | 2.52                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:1754:C:H5''  | 42:DT:113:LYS:NZ  | 2.31                     | 0.45              |
| 27:DA:200:U:H2'    | 27:DA:201:C:H5'   | 1.98                     | 0.45              |
| 27:DA:2027:G:O6    | 27:DA:2033:A:C8   | 2.70                     | 0.45              |
| 27:DA:2077:A:C5    | 27:DA:2435:A:C6   | 3.04                     | 0.45              |
| 27:DA:2392:A:P     | 57:D8:31:HIS:HE1  | 2.39                     | 0.45              |
| 27:DA:2697:G:H1    | 27:DA:2710:C:N4   | 2.14                     | 0.45              |
| 27:DA:272(I):U:H2' | 27:DA:272(J):C:C6 | 2.52                     | 0.45              |
| 27:DA:442:G:O2'    | 27:DA:443:A:OP1   | 2.32                     | 0.45              |
| 28:DB:6:C:H2'      | 28:DB:7:G:O4'     | 2.16                     | 0.45              |
| 29:DC:77:ILE:CG2   | 29:DC:123:VAL:H   | 2.26                     | 0.45              |
| 29:DC:67:GLY:O     | 29:DC:68:LEU:HB2  | 2.15                     | 0.45              |
| 32:DF:170:LEU:HD12 | 32:DF:171:PRO:HD3 | 1.99                     | 0.45              |
| 27:DA:2060:A:OP1   | 32:DF:68:LYS:O    | 2.34                     | 0.45              |
| 33:DG:6:ALA:HB3    | 33:DG:104:GLU:OE2 | 2.17                     | 0.45              |
| 33:DG:181:ARG:O    | 33:DG:182:LYS:C   | 2.55                     | 0.45              |
| 34:DH:116:GLU:HG2  | 34:DH:117:PRO:N   | 2.31                     | 0.45              |
| 38:DP:46:LYS:HG2   | 38:DP:52:GLU:OE2  | 2.16                     | 0.45              |
| 38:DP:7:ARG:O      | 38:DP:10:PRO:HD3  | 2.16                     | 0.45              |
| 39:DQ:137:TYR:H    | 39:DQ:137:TYR:HD2 | 1.63                     | 0.45              |
| 41:DS:62:LYS:O     | 41:DS:65:VAL:N    | 2.50                     | 0.45              |
| 42:DT:2:ASN:C      | 42:DT:3:ARG:HG2   | 2.37                     | 0.45              |
| 44:DV:39:LEU:HB3   | 44:DV:47:VAL:HG11 | 1.99                     | 0.45              |
| 45:DW:65:LEU:CD2   | 45:DW:67:ASP:H    | 2.29                     | 0.45              |
| 46:DX:8:ILE:HD11   | 46:DX:42:ALA:CB   | 2.47                     | 0.45              |
| 48:DZ:55:VAL:HG13  | 48:DZ:68:THR:O    | 2.16                     | 0.45              |
| 1:AA:113:G:H2'     | 1:AA:114:U:O5'    | 2.16                     | 0.45              |
| 1:AA:1393:U:H6     | 1:AA:1393:U:H3'   | 1.82                     | 0.45              |
| 1:AA:1406:U:C5     | 1:AA:1407:C:C5    | 3.05                     | 0.45              |
| 1:AA:228:A:H2'     | 1:AA:229:U:C6     | 2.52                     | 0.45              |
| 1:AA:279:A:H5''    | 1:AA:281:G:O4'    | 2.16                     | 0.45              |
| 1:AA:296:U:O2'     | 1:AA:297:G:H5'    | 2.15                     | 0.45              |
| 1:AA:389:A:C2'     | 1:AA:390:C:H5'    | 2.46                     | 0.45              |
| 1:AA:563:A:C2      | 1:AA:567:G:C5     | 3.04                     | 0.45              |
| 1:AA:618:C:H3'     | 1:AA:619:U:C5'    | 2.44                     | 0.45              |
| 2:AB:84:GLU:O      | 2:AB:219:VAL:HG21 | 2.16                     | 0.45              |
| 2:AB:35:GLU:C      | 2:AB:36:ARG:HE    | 2.20                     | 0.45              |
| 3:AC:115:LEU:O     | 3:AC:118:GLN:HB2  | 2.17                     | 0.45              |
| 4:AD:11:LEU:HD13   | 4:AD:66:ARG:HD3   | 1.97                     | 0.45              |
| 5:AE:76:ILE:HG23   | 5:AE:93:PRO:HB3   | 1.99                     | 0.45              |
| 6:AF:39:LYS:HG2    | 6:AF:40:VAL:N     | 2.32                     | 0.45              |
| 6:AF:19:LEU:HD11   | 6:AF:59:TYR:CD1   | 2.51                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:AH:82:HIS:N     | 8:AH:138:TRP:O     | 2.44                     | 0.45              |
| 8:AH:7:ALA:HA     | 8:AH:10:LEU:HD12   | 1.98                     | 0.45              |
| 9:AI:53:VAL:O     | 9:AI:54:ASP:CB     | 2.65                     | 0.45              |
| 10:AJ:29:ARG:NH2  | 10:AJ:84:GLN:HG2   | 2.31                     | 0.45              |
| 11:AK:34:ASP:HB2  | 11:AK:35:PRO:CD    | 2.47                     | 0.45              |
| 1:AA:1228:C:H4'   | 13:AM:116:THR:N    | 2.32                     | 0.45              |
| 18:AR:86:VAL:HG12 | 18:AR:87:ARG:HD2   | 1.98                     | 0.45              |
| 19:AS:61:TYR:O    | 19:AS:62:ILE:CG2   | 2.65                     | 0.45              |
| 20:AT:89:ARG:C    | 20:AT:91:LEU:H     | 2.18                     | 0.45              |
| 24:AX:62:C:H2'    | 24:AX:63:G:C8      | 2.51                     | 0.45              |
| 49:B0:41:ARG:N    | 49:B0:41:ARG:CD    | 2.80                     | 0.45              |
| 49:B0:41:ARG:O    | 49:B0:57:PHE:HD2   | 1.99                     | 0.45              |
| 52:B3:19:GLN:O    | 52:B3:23:LEU:CD1   | 2.64                     | 0.45              |
| 55:B6:16:CYS:SG   | 55:B6:48:VAL:HG21  | 2.57                     | 0.45              |
| 57:B8:22:VAL:HB   | 57:B8:49:VAL:CG2   | 2.47                     | 0.45              |
| 27:BA:1171:G:H5'' | 27:BA:1173:G:OP2   | 2.16                     | 0.45              |
| 27:BA:125:G:C5'   | 27:BA:126:A:OP2    | 2.60                     | 0.45              |
| 27:BA:1627:G:N1   | 27:BA:1640:C:C5    | 2.85                     | 0.45              |
| 27:BA:1674:G:H1'  | 27:BA:1676:A:N6    | 2.32                     | 0.45              |
| 27:BA:1779:U:H5   | 27:BA:1784:A:N7    | 2.12                     | 0.45              |
| 27:BA:1826:G:OP1  | 30:BD:224:ALA:HB2  | 2.16                     | 0.45              |
| 27:BA:1843:C:H5'  | 30:BD:253:GLN:HE22 | 1.76                     | 0.45              |
| 27:BA:2036:C:O2'  | 27:BA:2037:G:O5'   | 2.35                     | 0.45              |
| 27:BA:2320:A:C2   | 27:BA:2333:A:C8    | 3.04                     | 0.45              |
| 27:BA:2402:C:H41  | 27:BA:2415:G:N2    | 2.15                     | 0.45              |
| 27:BA:2745:C:N4   | 27:BA:2759:G:H1    | 2.15                     | 0.45              |
| 27:BA:657:U:OP2   | 27:BA:657:U:H6     | 1.99                     | 0.45              |
| 27:BA:843:G:C2    | 27:BA:936:C:C2     | 3.04                     | 0.45              |
| 27:BA:843:G:N2    | 27:BA:936:C:C2     | 2.85                     | 0.45              |
| 27:BA:856:C:H2'   | 27:BA:857:C:H6     | 1.81                     | 0.45              |
| 29:BC:59:ARG:N    | 29:BC:59:ARG:HD3   | 2.32                     | 0.45              |
| 27:BA:1565:C:P    | 30:BD:4:LYS:HZ2    | 2.40                     | 0.45              |
| 32:BF:3:GLU:O     | 32:BF:19:GLU:HB3   | 2.16                     | 0.45              |
| 32:BF:64:ILE:HG23 | 32:BF:65:TRP:N     | 2.31                     | 0.45              |
| 33:BG:28:VAL:C    | 33:BG:30:GLU:H     | 2.20                     | 0.45              |
| 34:BH:121:ILE:CG2 | 34:BH:122:THR:N    | 2.80                     | 0.45              |
| 37:BO:98:VAL:HG12 | 37:BO:117:LEU:HD22 | 1.97                     | 0.45              |
| 39:BQ:35:VAL:CG1  | 39:BQ:130:LYS:HB3  | 2.47                     | 0.45              |
| 40:BR:18:LEU:HA   | 40:BR:18:LEU:HD22  | 1.71                     | 0.45              |
| 42:BT:28:VAL:HG13 | 42:BT:46:GLU:CA    | 2.45                     | 0.45              |
| 43:BU:65:ILE:O    | 43:BU:67:ALA:N     | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:BU:92:ARG:CD   | 44:BV:11:GLN:NE2  | 2.80                     | 0.45              |
| 48:BZ:4:LEU:HD22  | 48:BZ:43:PHE:HA   | 1.97                     | 0.45              |
| 1:CA:1283:G:H2'   | 1:CA:1284:C:C6    | 2.52                     | 0.45              |
| 1:CA:1344:C:O5'   | 1:CA:1344:C:H6    | 1.99                     | 0.45              |
| 1:CA:184:G:H2'    | 1:CA:185:A:C8     | 2.40                     | 0.45              |
| 1:CA:280:C:H4'    | 1:CA:281:G:OP2    | 2.17                     | 0.45              |
| 1:CA:513:C:N3     | 1:CA:539:A:C2     | 2.83                     | 0.45              |
| 1:CA:502:G:C2     | 1:CA:544:G:C2     | 3.05                     | 0.45              |
| 1:CA:681:C:H2'    | 1:CA:682:G:H8     | 1.81                     | 0.45              |
| 1:CA:711:G:C2     | 1:CA:712:A:C4     | 3.05                     | 0.45              |
| 1:CA:720:C:N3     | 1:CA:721:G:C6     | 2.85                     | 0.45              |
| 3:CC:110:ASN:HA   | 3:CC:116:VAL:HG22 | 1.97                     | 0.45              |
| 3:CC:182:ILE:HG23 | 3:CC:202:ILE:C    | 2.37                     | 0.45              |
| 3:CC:84:ILE:HA    | 3:CC:87:LEU:CG    | 2.46                     | 0.45              |
| 4:CD:4:TYR:CD2    | 4:CD:5:ILE:N      | 2.85                     | 0.45              |
| 7:CG:44:TYR:C     | 7:CG:46:ALA:H     | 2.19                     | 0.45              |
| 7:CG:99:LEU:O     | 7:CG:100:ALA:C    | 2.55                     | 0.45              |
| 9:CI:8:GLY:HA2    | 9:CI:79:LEU:HB3   | 1.98                     | 0.45              |
| 11:CK:31:THR:OG1  | 11:CK:42:TRP:HB3  | 2.16                     | 0.45              |
| 12:CL:25:LYS:O    | 12:CL:26:GLY:C    | 2.55                     | 0.45              |
| 13:CM:40:ASN:HA   | 13:CM:41:PRO:HD3  | 1.76                     | 0.45              |
| 17:CQ:51:TYR:HE2  | 17:CQ:76:LEU:N    | 2.15                     | 0.45              |
| 19:CS:51:VAL:HG22 | 19:CS:71:LEU:HD13 | 1.99                     | 0.45              |
| 49:D0:68:GLU:OE2  | 49:D0:82:ARG:HB3  | 2.16                     | 0.45              |
| 51:D2:53:LEU:HA   | 51:D2:53:LEU:HD23 | 1.75                     | 0.45              |
| 53:D4:53:THR:O    | 53:D4:54:LYS:CG   | 2.59                     | 0.45              |
| 57:D8:32:LEU:O    | 57:D8:33:ASN:C    | 2.54                     | 0.45              |
| 27:DA:1158:C:O2'  | 27:DA:1159:U:H6   | 2.00                     | 0.45              |
| 27:DA:1701:A:C2'  | 27:DA:1702:G:H5'  | 2.47                     | 0.45              |
| 27:DA:1817:G:C2'  | 27:DA:1818:U:H5'  | 2.46                     | 0.45              |
| 27:DA:2437:U:H2'  | 27:DA:2438:U:H6   | 1.82                     | 0.45              |
| 27:DA:2496:C:OP2  | 39:DQ:82:ARG:NH2  | 2.49                     | 0.45              |
| 27:DA:2508:G:H2'  | 27:DA:2509:G:C8   | 2.51                     | 0.45              |
| 27:DA:2524:G:H2'  | 27:DA:2741:A:H2   | 1.80                     | 0.45              |
| 27:DA:2584:U:O2   | 27:DA:2585:U:C5   | 2.69                     | 0.45              |
| 27:DA:2667:C:H1'  | 34:DH:109:PHE:CE2 | 2.51                     | 0.45              |
| 27:DA:2714:G:H2'  | 27:DA:2715:C:C6   | 2.50                     | 0.45              |
| 27:DA:2727:G:C2   | 27:DA:2728:U:C4   | 3.04                     | 0.45              |
| 27:DA:461:C:C2'   | 27:DA:462:C:H5'   | 2.46                     | 0.45              |
| 27:DA:543:C:N4    | 27:DA:551:G:N1    | 2.50                     | 0.45              |
| 27:DA:778:G:H2'   | 27:DA:779:U:O4'   | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:910:A:C4     | 39:DQ:13:GLN:NE2   | 2.85                     | 0.45              |
| 29:DC:19:VAL:HG21  | 29:DC:22:ILE:HD11  | 1.99                     | 0.45              |
| 30:DD:119:ALA:CB   | 30:DD:130:ALA:HB3  | 2.47                     | 0.45              |
| 30:DD:146:GLU:HB2  | 30:DD:152:GLY:O    | 2.17                     | 0.45              |
| 31:DE:65:GLY:O     | 31:DE:67:PHE:N     | 2.49                     | 0.45              |
| 32:DF:198:ALA:O    | 32:DF:201:VAL:HG12 | 2.17                     | 0.45              |
| 33:DG:86:MET:N     | 33:DG:87:PRO:HD2   | 2.32                     | 0.45              |
| 34:DH:86:GLU:HB2   | 34:DH:132:ARG:NH1  | 2.32                     | 0.45              |
| 34:DH:17:VAL:O     | 34:DH:17:VAL:HG12  | 2.17                     | 0.45              |
| 35:DI:126:TYR:O    | 35:DI:139:GLN:HG3  | 2.16                     | 0.45              |
| 37:DO:6:THR:CG2    | 37:DO:7:TYR:N      | 2.78                     | 0.45              |
| 39:DQ:81:VAL:HG23  | 39:DQ:82:ARG:H     | 1.81                     | 0.45              |
| 40:DR:16:HIS:O     | 40:DR:19:ALA:N     | 2.49                     | 0.45              |
| 40:DR:36:THR:O     | 40:DR:37:THR:C     | 2.55                     | 0.45              |
| 40:DR:84:ALA:N     | 40:DR:85:PRO:CD    | 2.79                     | 0.45              |
| 42:DT:27:THR:O     | 42:DT:28:VAL:HB    | 2.16                     | 0.45              |
| 42:DT:33:LYS:HE3   | 42:DT:74:ARG:NH2   | 2.31                     | 0.45              |
| 42:DT:80:SER:OG    | 42:DT:81:PRO:CD    | 2.64                     | 0.45              |
| 27:DA:995:C:C2     | 43:DU:57:PHE:CD1   | 3.04                     | 0.45              |
| 43:DU:76:TYR:O     | 43:DU:78:THR:N     | 2.49                     | 0.45              |
| 47:DY:16:ALA:HA    | 47:DY:21:LYS:CD    | 2.47                     | 0.45              |
| 48:DZ:129:PRO:C    | 48:DZ:130:ARG:HG3  | 2.36                     | 0.45              |
| 48:DZ:143:LEU:HD12 | 48:DZ:147:ASP:O    | 2.17                     | 0.45              |
| 48:DZ:150:HIS:CG   | 48:DZ:169:THR:HG22 | 2.52                     | 0.45              |
| 48:DZ:38:VAL:CG2   | 48:DZ:43:PHE:HB2   | 2.43                     | 0.45              |
| 1:AA:1014:A:H3'    | 1:AA:1015:A:H8     | 1.82                     | 0.45              |
| 1:AA:1146:A:O2'    | 1:AA:1147:C:C5'    | 2.65                     | 0.45              |
| 1:AA:119:A:O2'     | 1:AA:120:A:OP2     | 2.25                     | 0.45              |
| 1:AA:1420:C:O2'    | 1:AA:1421:G:H5'    | 2.17                     | 0.45              |
| 1:AA:1466:C:O2'    | 1:AA:1467:G:H5'    | 2.16                     | 0.45              |
| 1:AA:23:C:O2'      | 1:AA:24:U:H5'      | 2.17                     | 0.45              |
| 1:AA:60:A:O2'      | 1:AA:61:G:OP2      | 2.29                     | 0.45              |
| 1:AA:1058:G:H5'    | 3:AC:186:PHE:CE1   | 2.51                     | 0.45              |
| 3:AC:62:ASP:O      | 3:AC:98:ASN:HB3    | 2.17                     | 0.45              |
| 7:AG:27:ILE:O      | 7:AG:30:ILE:N      | 2.33                     | 0.45              |
| 7:AG:65:ALA:O      | 7:AG:69:VAL:HG23   | 2.17                     | 0.45              |
| 7:AG:95:ARG:HG2    | 7:AG:99:LEU:HD11   | 1.97                     | 0.45              |
| 9:AI:53:VAL:O      | 9:AI:54:ASP:HB2    | 2.17                     | 0.45              |
| 9:AI:95:LYS:HG3    | 9:AI:96:LEU:N      | 2.32                     | 0.45              |
| 10:AJ:81:THR:HA    | 10:AJ:84:GLN:OE1   | 2.17                     | 0.45              |
| 12:AL:25:LYS:O     | 12:AL:27:ALA:N     | 2.50                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1308:U:OP1    | 13:AM:97:PRO:HA   | 2.17                     | 0.45              |
| 10:AJ:62:HIS:CE1   | 14:AN:61:TRP:CH2  | 3.05                     | 0.45              |
| 15:AO:25:THR:O     | 15:AO:26:GLU:C    | 2.55                     | 0.45              |
| 13:AM:84:ILE:CG2   | 19:AS:74:PHE:HD1  | 2.29                     | 0.45              |
| 21:AU:3:LYS:O      | 21:AU:11:GLY:HA2  | 2.17                     | 0.45              |
| 25:AY:66:A:C2      | 25:AY:67:C:C2     | 3.05                     | 0.45              |
| 49:B0:19:LYS:HA    | 49:B0:19:LYS:HD2  | 1.88                     | 0.45              |
| 49:B0:46:LYS:HE3   | 49:B0:76:GLY:HA3  | 1.98                     | 0.45              |
| 51:B2:32:LEU:CA    | 51:B2:53:LEU:HD12 | 2.47                     | 0.45              |
| 27:BA:1030:G:C2'   | 27:BA:1031:G:O5'  | 2.64                     | 0.45              |
| 27:BA:1114:G:H3'   | 27:BA:1115:G:C5'  | 2.40                     | 0.45              |
| 27:BA:1317:A:C6    | 27:BA:1336:A:N1   | 2.85                     | 0.45              |
| 27:BA:1434:A:N6    | 27:BA:1558:A:N6   | 2.47                     | 0.45              |
| 27:BA:1665:A:C2'   | 27:BA:1666:G:H5'  | 2.45                     | 0.45              |
| 27:BA:1739:U:O4'   | 27:BA:1739:U:O2   | 2.35                     | 0.45              |
| 27:BA:1818:U:O2'   | 30:BD:155:LEU:HA  | 2.17                     | 0.45              |
| 27:BA:1892:C:H2'   | 27:BA:1893:C:H5'  | 1.99                     | 0.45              |
| 27:BA:2337:G:C2    | 27:BA:2338:G:N7   | 2.85                     | 0.45              |
| 27:BA:2420:C:OP1   | 57:B8:33:ASN:O    | 2.35                     | 0.45              |
| 27:BA:271(J):C:N3  | 27:BA:271(M):G:O6 | 2.50                     | 0.45              |
| 27:BA:2805:G:H2'   | 27:BA:2807:G:H5'' | 1.99                     | 0.45              |
| 27:BA:309:G:N3     | 27:BA:329:G:O2'   | 2.47                     | 0.45              |
| 27:BA:467:G:O2'    | 27:BA:468:G:H5'   | 2.17                     | 0.45              |
| 27:BA:533:G:C5     | 27:BA:561:G:N2    | 2.85                     | 0.45              |
| 27:BA:819:A:O2'    | 27:BA:820:A:H5'   | 2.17                     | 0.45              |
| 27:BA:838:C:C4     | 27:BA:839:U:C5    | 3.05                     | 0.45              |
| 27:BA:860:U:H2'    | 27:BA:861:A:C8    | 2.52                     | 0.45              |
| 28:BB:3:C:C4       | 28:BB:4:C:C5      | 3.04                     | 0.45              |
| 27:BA:1812:A:O2'   | 30:BD:45:ASN:HB2  | 2.17                     | 0.45              |
| 32:BF:3:GLU:HB3    | 32:BF:24:LEU:HG   | 1.98                     | 0.45              |
| 33:BG:147:ASP:OD1  | 33:BG:148:MET:N   | 2.50                     | 0.45              |
| 33:BG:176:LEU:HD12 | 33:BG:176:LEU:N   | 2.32                     | 0.45              |
| 34:BH:44:VAL:O     | 34:BH:46:GLU:OE2  | 2.35                     | 0.45              |
| 34:BH:8:PRO:CD     | 34:BH:65:HIS:HE1  | 2.29                     | 0.45              |
| 35:BI:42:SER:O     | 35:BI:44:LEU:N    | 2.50                     | 0.45              |
| 39:BQ:118:LEU:HD23 | 39:BQ:118:LEU:HA  | 1.74                     | 0.45              |
| 40:BR:79:LEU:HA    | 40:BR:83:ILE:CB   | 2.47                     | 0.45              |
| 42:BT:85:LYS:C     | 42:BT:85:LYS:HZ1  | 2.19                     | 0.45              |
| 42:BT:28:VAL:HB    | 42:BT:88:ILE:HD12 | 1.97                     | 0.45              |
| 42:BT:96:ARG:HB3   | 42:BT:96:ARG:HE   | 1.55                     | 0.45              |
| 27:BA:1754:C:P     | 42:BT:96:ARG:HH12 | 2.38                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:BU:98:LEU:HA   | 43:BU:101:ARG:O   | 2.16                     | 0.45              |
| 43:BU:71:GLN:C    | 43:BU:72:HIS:CD2  | 2.90                     | 0.45              |
| 43:BU:66:ASN:HA   | 43:BU:76:TYR:HB2  | 1.99                     | 0.45              |
| 43:BU:77:SER:OG   | 43:BU:78:THR:N    | 2.49                     | 0.45              |
| 44:BV:5:VAL:HG13  | 44:BV:14:VAL:CG2  | 2.47                     | 0.45              |
| 27:BA:310:A:OP1   | 47:BY:17:SER:O    | 2.35                     | 0.45              |
| 47:BY:31:LEU:CD2  | 47:BY:31:LEU:N    | 2.78                     | 0.45              |
| 47:BY:42:VAL:C    | 47:BY:65:ALA:HB3  | 2.37                     | 0.45              |
| 1:CA:1061:G:H1'   | 10:CJ:56:HIS:CE1  | 2.51                     | 0.45              |
| 1:CA:1165:C:H42   | 1:CA:1172:C:H42   | 1.63                     | 0.45              |
| 1:CA:117:G:O5'    | 1:CA:117:G:H8     | 1.99                     | 0.45              |
| 1:CA:1229:A:H2'   | 1:CA:1230:C:C6    | 2.52                     | 0.45              |
| 1:CA:1502:A:C2    | 1:CA:1505:G:N1    | 2.57                     | 0.45              |
| 1:CA:31:G:N2      | 1:CA:47:C:H4'     | 2.32                     | 0.45              |
| 1:CA:537:G:H8     | 1:CA:537:G:O5'    | 1.99                     | 0.45              |
| 1:CA:56:U:H2'     | 1:CA:56:U:O2      | 2.16                     | 0.45              |
| 1:CA:832:C:C2'    | 1:CA:833:U:H5'    | 2.47                     | 0.45              |
| 1:CA:663:A:H5'    | 1:CA:836:G:OP1    | 2.17                     | 0.45              |
| 2:CB:115:LEU:O    | 2:CB:115:LEU:HD12 | 2.16                     | 0.45              |
| 4:CD:24:GLU:O     | 4:CD:27:TYR:HB2   | 2.16                     | 0.45              |
| 4:CD:3:ARG:HH21   | 4:CD:5:ILE:HD11   | 1.82                     | 0.45              |
| 5:CE:42:GLY:CA    | 5:CE:65:ASN:O     | 2.60                     | 0.45              |
| 7:CG:42:ILE:HD13  | 7:CG:116:ALA:HB1  | 1.98                     | 0.45              |
| 7:CG:22:LEU:HD23  | 7:CG:62:PHE:HE2   | 1.82                     | 0.45              |
| 9:CI:65:VAL:HG13  | 9:CI:73:GLN:NE2   | 2.32                     | 0.45              |
| 11:CK:38:ASN:HA   | 11:CK:39:PRO:HD3  | 1.87                     | 0.45              |
| 15:CO:76:GLU:HA   | 15:CO:76:GLU:OE1  | 2.16                     | 0.45              |
| 16:CP:19:ILE:HG22 | 16:CP:36:ILE:HD11 | 1.98                     | 0.45              |
| 18:CR:82:THR:CG2  | 18:CR:83:GLU:N    | 2.64                     | 0.45              |
| 19:CS:25:LYS:HB3  | 19:CS:27:GLU:OE1  | 2.16                     | 0.45              |
| 20:CT:26:ASN:CB   | 20:CT:71:THR:HG23 | 2.28                     | 0.45              |
| 23:CW:22:G:H2'    | 23:CW:23:G:H8     | 1.81                     | 0.45              |
| 23:CW:28:G:O6     | 23:CW:40:C:N3     | 2.50                     | 0.45              |
| 23:CW:7:A:C2      | 23:CW:66:A:C2     | 3.04                     | 0.45              |
| 49:D0:32:ARG:HB2  | 49:D0:35:ASN:OD1  | 2.16                     | 0.45              |
| 50:D1:43:TYR:HA   | 50:D1:44:PRO:HD3  | 1.78                     | 0.45              |
| 52:D3:23:LEU:HD11 | 52:D3:50:VAL:HG11 | 1.99                     | 0.45              |
| 52:D3:39:ASP:OD1  | 52:D3:44:ARG:NE   | 2.49                     | 0.45              |
| 54:D5:52:TYR:O    | 54:D5:53:ALA:C    | 2.55                     | 0.45              |
| 27:DA:1034:G:O2'  | 27:DA:1035:U:O4'  | 2.34                     | 0.45              |
| 27:DA:1037:G:N2   | 27:DA:1119:C:C2   | 2.85                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1208:C:C2'   | 27:DA:1209:G:H5'   | 2.47                     | 0.45              |
| 27:DA:1288:U:H4'   | 27:DA:1289:C:OP2   | 2.16                     | 0.45              |
| 27:DA:1579:A:H2'   | 27:DA:1580:A:C8    | 2.52                     | 0.45              |
| 27:DA:1876:A:H3'   | 27:DA:1877:A:H8    | 1.82                     | 0.45              |
| 27:DA:1917:U:H2'   | 27:DA:1918:A:O4'   | 2.17                     | 0.45              |
| 27:DA:1661:G:C4    | 27:DA:2000:G:N2    | 2.85                     | 0.45              |
| 27:DA:2152:G:H2'   | 27:DA:2153:G:C8    | 2.34                     | 0.45              |
| 27:DA:2261:C:P     | 49:D0:17:GLN:OE1   | 2.75                     | 0.45              |
| 27:DA:2743:C:H2'   | 27:DA:2744:G:O5'   | 2.16                     | 0.45              |
| 27:DA:718:A:H2'    | 27:DA:719:C:H5'    | 1.99                     | 0.45              |
| 27:DA:779:U:C4     | 27:DA:780:G:C5     | 3.05                     | 0.45              |
| 27:DA:794:G:C6     | 27:DA:795:C:C4     | 3.04                     | 0.45              |
| 27:DA:918:A:H1'    | 28:DB:80:U:O2'     | 2.17                     | 0.45              |
| 28:DB:43:C:C4      | 28:DB:45:A:C6      | 3.04                     | 0.45              |
| 30:DD:105:ILE:HD12 | 30:DD:105:ILE:HA   | 1.64                     | 0.45              |
| 30:DD:213:ARG:HD3  | 30:DD:218:ARG:HA   | 1.98                     | 0.45              |
| 30:DD:43:ARG:HB2   | 30:DD:54:ARG:HB2   | 1.98                     | 0.45              |
| 31:DE:76:ARG:CG    | 31:DE:195:LEU:HD13 | 2.40                     | 0.45              |
| 33:DG:131:TYR:O    | 33:DG:159:VAL:CG1  | 2.65                     | 0.45              |
| 33:DG:5:VAL:HG23   | 33:DG:8:LYS:CG     | 2.35                     | 0.45              |
| 35:DI:79:ILE:O     | 35:DI:143:SER:N    | 2.39                     | 0.45              |
| 27:DA:1141:U:OP1   | 36:DN:25:ARG:NH1   | 2.50                     | 0.45              |
| 36:DN:67:LEU:H     | 36:DN:67:LEU:HD12  | 1.82                     | 0.45              |
| 27:DA:1287:A:O4'   | 40:DR:104:ARG:NH2  | 2.49                     | 0.45              |
| 42:DT:109:GLU:HG2  | 42:DT:112:ARG:HH12 | 1.80                     | 0.45              |
| 42:DT:64:ARG:HG3   | 42:DT:72:VAL:O     | 2.17                     | 0.45              |
| 44:DV:19:LYS:HZ3   | 44:DV:20:LEU:HB2   | 1.82                     | 0.45              |
| 44:DV:45:THR:O     | 44:DV:46:VAL:HG12  | 2.16                     | 0.45              |
| 45:DW:3:ALA:HB2    | 45:DW:62:HIS:ND1   | 2.32                     | 0.45              |
| 45:DW:44:ALA:O     | 45:DW:45:TYR:C     | 2.54                     | 0.45              |
| 47:DY:25:GLY:HA3   | 47:DY:40:GLU:HG2   | 1.99                     | 0.45              |
| 47:DY:95:LYS:CE    | 47:DY:100:ALA:HB2  | 2.47                     | 0.45              |
| 1:AA:1264:C:C6     | 1:AA:1264:C:C3'    | 2.99                     | 0.45              |
| 1:AA:1275:A:O2'    | 1:AA:1276:G:H5'    | 2.17                     | 0.45              |
| 1:AA:1321:C:H3'    | 1:AA:1322:C:H5''   | 1.99                     | 0.45              |
| 1:AA:502:G:OP1     | 12:AL:115:SER:N    | 2.25                     | 0.45              |
| 1:AA:57:G:C8       | 1:AA:58:C:C5       | 3.05                     | 0.45              |
| 1:AA:667:G:O2'     | 1:AA:668:G:H5'     | 2.17                     | 0.45              |
| 1:AA:657:G:C2      | 1:AA:750:G:C5      | 3.05                     | 0.45              |
| 1:AA:9:G:H5''      | 5:AE:122:GLU:OE1   | 2.17                     | 0.45              |
| 2:AB:97:TRP:CH2    | 2:AB:173:ALA:HA    | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:236:TYR:CG   | 2:AB:239:VAL:HG21 | 2.51                     | 0.45              |
| 2:AB:45:GLN:O     | 2:AB:48:MET:HB3   | 2.17                     | 0.45              |
| 1:AA:1205:U:OP1   | 3:AC:190:ARG:NH2  | 2.49                     | 0.45              |
| 3:AC:87:LEU:O     | 3:AC:89:GLU:N     | 2.50                     | 0.45              |
| 3:AC:90:GLU:O     | 3:AC:93:LYS:CB    | 2.65                     | 0.45              |
| 4:AD:104:VAL:HA   | 4:AD:107:ARG:HB2  | 1.99                     | 0.45              |
| 4:AD:105:VAL:O    | 4:AD:105:VAL:HG12 | 2.17                     | 0.45              |
| 6:AF:6:VAL:CG1    | 6:AF:90:VAL:HG22  | 2.47                     | 0.45              |
| 7:AG:127:ALA:C    | 7:AG:129:GLU:N    | 2.68                     | 0.45              |
| 8:AH:18:ARG:NH2   | 8:AH:81:HIS:O     | 2.49                     | 0.45              |
| 10:AJ:98:ILE:O    | 10:AJ:98:ILE:HG22 | 2.17                     | 0.45              |
| 1:AA:1225:A:H5''  | 13:AM:103:THR:OG1 | 2.17                     | 0.45              |
| 13:AM:91:ARG:NH1  | 13:AM:96:LEU:HD13 | 2.32                     | 0.45              |
| 13:AM:91:ARG:NH1  | 19:AS:81:ARG:HH22 | 2.14                     | 0.45              |
| 15:AO:3:ILE:O     | 15:AO:3:ILE:HG13  | 2.16                     | 0.45              |
| 15:AO:5:LYS:HB3   | 15:AO:5:LYS:HE2   | 1.84                     | 0.45              |
| 15:AO:74:ASP:O    | 15:AO:75:PRO:C    | 2.55                     | 0.45              |
| 12:AL:5:ASN:ND2   | 17:AQ:34:LYS:HE2  | 2.31                     | 0.45              |
| 1:AA:264:U:O2'    | 17:AQ:64:PRO:O    | 2.34                     | 0.45              |
| 17:AQ:81:ARG:O    | 17:AQ:83:ASP:N    | 2.50                     | 0.45              |
| 20:AT:24:LEU:O    | 20:AT:27:LYS:N    | 2.47                     | 0.45              |
| 49:B0:43:THR:CG2  | 49:B0:43:THR:O    | 2.64                     | 0.45              |
| 55:B6:52:VAL:HG12 | 55:B6:52:VAL:O    | 2.17                     | 0.45              |
| 56:B7:23:ARG:O    | 56:B7:28:ARG:CZ   | 2.65                     | 0.45              |
| 27:BA:107:C:O5'   | 27:BA:107:C:H6    | 2.00                     | 0.45              |
| 27:BA:1179:C:H2'  | 27:BA:1180:C:C6   | 2.50                     | 0.45              |
| 27:BA:1298:C:N4   | 27:BA:1299:G:C6   | 2.84                     | 0.45              |
| 27:BA:1354:A:H2'  | 27:BA:1355:G:O4'  | 2.17                     | 0.45              |
| 27:BA:1384:A:H1'  | 27:BA:1405:U:O4'  | 2.17                     | 0.45              |
| 27:BA:1427:A:H4'  | 27:BA:1428:C:O5'  | 2.16                     | 0.45              |
| 27:BA:146:G:H2'   | 27:BA:147:U:H5'   | 1.99                     | 0.45              |
| 27:BA:1718:G:C2   | 27:BA:1745:C:C2   | 3.04                     | 0.45              |
| 27:BA:530:G:C5    | 27:BA:2022:U:H5'' | 2.52                     | 0.45              |
| 27:BA:2041:U:H2'  | 27:BA:2042:A:O4'  | 2.16                     | 0.45              |
| 27:BA:2488:A:H2'  | 27:BA:2489:G:H8   | 1.79                     | 0.45              |
| 27:BA:251:A:C5    | 27:BA:252:G:H1'   | 2.52                     | 0.45              |
| 27:BA:2543:G:H5'  | 27:BA:2543:G:C8   | 2.42                     | 0.45              |
| 27:BA:2857:G:H5'' | 27:BA:2858:C:OP2  | 2.16                     | 0.45              |
| 27:BA:838:C:H2'   | 27:BA:839:U:C6    | 2.45                     | 0.45              |
| 27:BA:838:C:C2    | 27:BA:839:U:C5    | 3.05                     | 0.45              |
| 27:BA:863:A:H3'   | 39:BQ:22:LYS:HD2  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:867:C:O2    | 27:BA:913:U:H5'   | 2.16                     | 0.45              |
| 30:BD:146:GLU:CB  | 30:BD:189:CYS:HB3 | 2.47                     | 0.45              |
| 27:BA:1997:G:OP1  | 31:BE:123:ALA:HA  | 2.17                     | 0.45              |
| 27:BA:2580:U:C4'  | 31:BE:131:ALA:H   | 2.28                     | 0.45              |
| 31:BE:144:ARG:HB3 | 31:BE:145:LYS:H   | 1.45                     | 0.45              |
| 33:BG:123:ASN:O   | 33:BG:126:ASP:CG  | 2.55                     | 0.45              |
| 34:BH:82:GLY:O    | 34:BH:83:TYR:C    | 2.55                     | 0.45              |
| 37:BO:14:THR:CG2  | 37:BO:16:ALA:H    | 2.28                     | 0.45              |
| 39:BQ:5:ARG:O     | 39:BQ:6:ARG:CB    | 2.65                     | 0.45              |
| 41:BS:54:LEU:HD11 | 41:BS:59:LYS:O    | 2.17                     | 0.45              |
| 44:BV:21:ARG:NH1  | 44:BV:91:TYR:CE2  | 2.85                     | 0.45              |
| 46:BX:64:LYS:HZ3  | 46:BX:73:ARG:NE   | 1.87                     | 0.45              |
| 46:BX:47:PHE:CD2  | 46:BX:89:ILE:HD13 | 2.52                     | 0.45              |
| 48:BZ:52:ILE:HG22 | 48:BZ:70:VAL:O    | 2.17                     | 0.45              |
| 1:CA:1262:C:H2'   | 1:CA:1263:C:C6    | 2.52                     | 0.45              |
| 1:CA:1341:U:O2'   | 1:CA:1342:C:H5'   | 2.17                     | 0.45              |
| 1:CA:815:A:N6     | 1:CA:1509:C:H1'   | 2.32                     | 0.45              |
| 1:CA:198:G:C2     | 1:CA:199:G:C4     | 3.05                     | 0.45              |
| 1:CA:236:G:O2'    | 1:CA:237:C:H5'    | 2.17                     | 0.45              |
| 1:CA:301:G:H2'    | 1:CA:302:G:H8     | 1.82                     | 0.45              |
| 1:CA:35:G:C2      | 1:CA:550:G:N3     | 2.85                     | 0.45              |
| 1:CA:511:C:H2'    | 1:CA:534:U:O2     | 2.17                     | 0.45              |
| 1:CA:593:G:C2     | 1:CA:594:G:C4     | 3.05                     | 0.45              |
| 1:CA:602:A:N6     | 1:CA:637:G:C6     | 2.85                     | 0.45              |
| 1:CA:806:C:H2'    | 1:CA:807:A:C8     | 2.51                     | 0.45              |
| 1:CA:862:C:N3     | 1:CA:863:U:C5     | 2.85                     | 0.45              |
| 1:CA:937:A:H62    | 1:CA:938:A:N6     | 2.14                     | 0.45              |
| 1:CA:983:A:C2'    | 1:CA:984:C:H5'    | 2.47                     | 0.45              |
| 2:CB:134:GLU:O    | 2:CB:138:LEU:HG   | 2.17                     | 0.45              |
| 3:CC:126:ARG:HG2  | 3:CC:126:ARG:HH11 | 1.81                     | 0.45              |
| 3:CC:180:ALA:HB1  | 3:CC:182:ILE:CD1  | 2.46                     | 0.45              |
| 4:CD:173:TRP:CA   | 4:CD:187:ARG:NH1  | 2.79                     | 0.45              |
| 4:CD:79:PHE:CD2   | 4:CD:80:GLU:N     | 2.84                     | 0.45              |
| 6:CF:44:GLY:O     | 6:CF:45:LEU:O     | 2.35                     | 0.45              |
| 10:CJ:30:SER:CB   | 10:CJ:80:LYS:HD3  | 2.47                     | 0.45              |
| 10:CJ:85:LEU:C    | 10:CJ:87:THR:H    | 2.19                     | 0.45              |
| 17:CQ:11:VAL:HG11 | 17:CQ:88:TYR:HD2  | 1.81                     | 0.45              |
| 17:CQ:10:VAL:CG1  | 17:CQ:19:VAL:HB   | 2.47                     | 0.45              |
| 21:CU:18:TYR:HD2  | 21:CU:22:ARG:HD3  | 1.81                     | 0.45              |
| 51:D2:43:GLN:HG3  | 51:D2:43:GLN:O    | 2.16                     | 0.45              |
| 56:D7:8:ASN:ND2   | 56:D7:10:ARG:N    | 2.65                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:1204:A:C8   | 27:DA:1206:G:C6    | 3.05                     | 0.45              |
| 27:DA:1256:G:N3   | 27:DA:1256:G:H2'   | 2.31                     | 0.45              |
| 27:DA:1345:C:H2'  | 27:DA:1346:G:H8    | 1.81                     | 0.45              |
| 27:DA:1639:U:C2'  | 27:DA:1640:C:C5'   | 2.93                     | 0.45              |
| 27:DA:1668:A:C8   | 27:DA:1674:G:C6    | 3.05                     | 0.45              |
| 27:DA:1130:U:C2   | 27:DA:2025:C:H5''  | 2.52                     | 0.45              |
| 27:DA:2327:A:H2'  | 27:DA:2328:A:H8    | 1.76                     | 0.45              |
| 27:DA:2343:C:O2'  | 27:DA:2373:G:H4'   | 2.17                     | 0.45              |
| 27:DA:2447:G:C2   | 27:DA:2501:C:N4    | 2.85                     | 0.45              |
| 27:DA:2483:C:N3   | 39:DQ:124:LYS:NZ   | 2.56                     | 0.45              |
| 27:DA:2629:A:N3   | 27:DA:2629:A:C5'   | 2.76                     | 0.45              |
| 27:DA:271(H):G:H1 | 27:DA:271(P):C:H42 | 1.63                     | 0.45              |
| 27:DA:354:G:H2'   | 27:DA:355:G:H8     | 1.82                     | 0.45              |
| 27:DA:36:G:N2     | 27:DA:37:C:H1'     | 2.32                     | 0.45              |
| 27:DA:431:U:O2'   | 27:DA:432:A:H5'    | 2.16                     | 0.45              |
| 27:DA:308:G:C8    | 27:DA:501:A:H1'    | 2.52                     | 0.45              |
| 27:DA:84:A:C2     | 27:DA:98:G:N3      | 2.85                     | 0.45              |
| 27:DA:864:G:C6    | 27:DA:865:C:H5     | 2.34                     | 0.45              |
| 27:DA:932:G:O2'   | 27:DA:933:A:OP2    | 2.29                     | 0.45              |
| 27:DA:995:C:C2    | 36:DN:4:TYR:OH     | 2.68                     | 0.45              |
| 27:DA:862:G:N2    | 28:DB:101:G:H1'    | 2.32                     | 0.45              |
| 30:DD:208:LYS:HE3 | 30:DD:208:LYS:HB2  | 1.84                     | 0.45              |
| 30:DD:65:ILE:CD1  | 30:DD:65:ILE:N     | 2.74                     | 0.45              |
| 31:DE:4:ILE:CG2   | 31:DE:4:ILE:O      | 2.63                     | 0.45              |
| 27:DA:675:A:H5'   | 32:DF:63:LYS:CE    | 2.47                     | 0.45              |
| 33:DG:39:ILE:HD12 | 33:DG:40:ASN:H     | 1.82                     | 0.45              |
| 33:DG:55:LYS:O    | 33:DG:55:LYS:HD3   | 2.16                     | 0.45              |
| 34:DH:65:HIS:O    | 34:DH:69:ARG:HB2   | 2.17                     | 0.45              |
| 35:DI:92:VAL:HG23 | 35:DI:96:ASP:HB2   | 1.98                     | 0.45              |
| 37:DO:3:GLN:HB2   | 37:DO:4:PRO:HD2    | 1.99                     | 0.45              |
| 38:DP:115:LEU:HB2 | 38:DP:131:SER:OG   | 2.17                     | 0.45              |
| 38:DP:18:ARG:O    | 38:DP:20:GLY:N     | 2.50                     | 0.45              |
| 39:DQ:111:GLU:CD  | 39:DQ:133:ARG:HH21 | 2.17                     | 0.45              |
| 41:DS:88:ASP:OD2  | 41:DS:89:ARG:N     | 2.50                     | 0.45              |
| 42:DT:89:VAL:HB   | 42:DT:91:ARG:NE    | 2.32                     | 0.45              |
| 43:DU:85:LYS:C    | 43:DU:87:GLY:N     | 2.69                     | 0.45              |
| 44:DV:19:LYS:NZ   | 44:DV:20:LEU:C     | 2.70                     | 0.45              |
| 27:DA:1187:G:H5'' | 44:DV:81:TYR:CZ    | 2.52                     | 0.45              |
| 44:DV:73:SER:HB2  | 44:DV:83:ARG:O     | 2.17                     | 0.45              |
| 27:DA:495:G:N2    | 45:DW:61:ASN:HD21  | 2.14                     | 0.45              |
| 46:DX:44:GLU:C    | 46:DX:46:ALA:H     | 2.18                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:DZ:114:GLY:HA2 | 48:DZ:173:VAL:CG1 | 2.47                     | 0.45              |
| 48:DZ:3:ARG:CG    | 48:DZ:57:VAL:HB   | 2.47                     | 0.45              |
| 1:AA:1136:U:H6    | 1:AA:1136:U:O5'   | 1.99                     | 0.45              |
| 1:AA:1057:G:N2    | 1:AA:1204:A:H1'   | 2.32                     | 0.45              |
| 1:AA:1267:C:O2    | 1:AA:1267:C:H2'   | 2.17                     | 0.45              |
| 1:AA:1495:U:H6    | 1:AA:1495:U:O5'   | 1.99                     | 0.45              |
| 1:AA:183:G:H2'    | 1:AA:184:G:C8     | 2.52                     | 0.45              |
| 1:AA:226:G:N3     | 1:AA:226:G:H2'    | 2.30                     | 0.45              |
| 1:AA:506:G:C5     | 1:AA:507:C:C5     | 3.05                     | 0.45              |
| 1:AA:55:A:O2'     | 1:AA:56:U:H5'     | 2.17                     | 0.45              |
| 1:AA:606:G:H2'    | 1:AA:631:G:H1     | 1.80                     | 0.45              |
| 1:AA:664:G:OP1    | 18:AR:64:ARG:NH2  | 2.46                     | 0.45              |
| 1:AA:714:G:O2'    | 1:AA:715:A:H5'    | 2.17                     | 0.45              |
| 2:AB:155:LEU:HD13 | 2:AB:156:LYS:N    | 2.31                     | 0.45              |
| 3:AC:131:ARG:HH12 | 3:AC:135:LYS:HE3  | 1.82                     | 0.45              |
| 3:AC:155:GLY:O    | 3:AC:196:LEU:HD13 | 2.16                     | 0.45              |
| 4:AD:100:ARG:NH2  | 4:AD:118:ARG:NH2  | 2.65                     | 0.45              |
| 5:AE:118:ILE:HG13 | 5:AE:119:LEU:N    | 2.31                     | 0.45              |
| 6:AF:67:MET:CB    | 6:AF:68:PRO:HD2   | 2.34                     | 0.45              |
| 10:AJ:46:ARG:CG   | 10:AJ:64:GLU:OE1  | 2.55                     | 0.45              |
| 13:AM:7:VAL:HG12  | 13:AM:9:ILE:CD1   | 2.38                     | 0.45              |
| 16:AP:55:ARG:O    | 16:AP:56:ALA:C    | 2.55                     | 0.45              |
| 20:AT:43:LEU:HB3  | 20:AT:48:LYS:CG   | 2.46                     | 0.45              |
| 20:AT:88:VAL:O    | 20:AT:91:LEU:HB2  | 2.17                     | 0.45              |
| 23:AW:59:U:H5''   | 23:AW:60:C:H5     | 1.82                     | 0.45              |
| 24:AX:19:G:H5'    | 24:AX:20:U:C6     | 2.51                     | 0.45              |
| 55:B6:20:ASN:C    | 55:B6:21:TYR:CG   | 2.89                     | 0.45              |
| 27:BA:1375:C:H2'  | 27:BA:1376:C:C6   | 2.48                     | 0.45              |
| 27:BA:1386:C:H2'  | 27:BA:1387:C:C5   | 2.52                     | 0.45              |
| 27:BA:1406:U:H2'  | 27:BA:1407:C:H6   | 1.79                     | 0.45              |
| 27:BA:1490:A:C2'  | 27:BA:1490:A:N3   | 2.77                     | 0.45              |
| 27:BA:1702:G:H2'  | 27:BA:1703:G:O4'  | 2.16                     | 0.45              |
| 27:BA:2199:A:H3'  | 27:BA:2200:C:H5'' | 1.98                     | 0.45              |
| 27:BA:2313:C:C4   | 27:BA:2314:C:C5   | 3.05                     | 0.45              |
| 27:BA:2302:G:C6   | 27:BA:2315:G:C6   | 3.06                     | 0.45              |
| 27:BA:248:G:C2    | 27:BA:2431:U:H4'  | 2.52                     | 0.45              |
| 27:BA:2445:G:C2'  | 27:BA:2446:G:H5'  | 2.47                     | 0.45              |
| 27:BA:2525:G:N3   | 27:BA:2525:G:H2'  | 2.32                     | 0.45              |
| 27:BA:2803:C:H2'  | 27:BA:2804:C:C5   | 2.52                     | 0.45              |
| 27:BA:291:C:H2'   | 27:BA:292:C:H6    | 1.82                     | 0.45              |
| 27:BA:332:A:C2    | 27:BA:335:C:C5    | 3.04                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:638:G:C6    | 27:BA:639:U:N3    | 2.85                     | 0.45              |
| 27:BA:722:A:N6    | 27:BA:723:G:C6    | 2.85                     | 0.45              |
| 27:BA:81:G:H2'    | 27:BA:82:G:O4'    | 2.17                     | 0.45              |
| 27:BA:1824:G:O3'  | 30:BD:249:PRO:HD3 | 2.17                     | 0.45              |
| 27:BA:1813:G:O4'  | 30:BD:45:ASN:HB3  | 2.16                     | 0.45              |
| 31:BE:47:VAL:HG12 | 31:BE:48:GLN:N    | 2.32                     | 0.45              |
| 31:BE:51:PHE:O    | 31:BE:52:LEU:HB2  | 2.17                     | 0.45              |
| 31:BE:52:LEU:HD12 | 31:BE:52:LEU:HA   | 1.74                     | 0.45              |
| 32:BF:3:GLU:C     | 32:BF:19:GLU:CB   | 2.85                     | 0.45              |
| 32:BF:64:ILE:HG23 | 32:BF:65:TRP:CD1  | 2.52                     | 0.45              |
| 34:BH:45:VAL:O    | 34:BH:45:VAL:CG1  | 2.59                     | 0.45              |
| 35:BI:83:ALA:CB   | 35:BI:88:ILE:HA   | 2.47                     | 0.45              |
| 35:BI:92:VAL:O    | 35:BI:93:THR:C    | 2.55                     | 0.45              |
| 36:BN:73:THR:CG2  | 36:BN:74:ARG:N    | 2.80                     | 0.45              |
| 38:BP:96:THR:HG22 | 38:BP:126:VAL:HB  | 1.99                     | 0.45              |
| 40:BR:63:ARG:HA   | 40:BR:80:PHE:CZ   | 2.51                     | 0.45              |
| 41:BS:96:GLY:C    | 41:BS:98:VAL:H    | 2.20                     | 0.45              |
| 42:BT:12:SER:O    | 42:BT:13:ARG:NH1  | 2.49                     | 0.45              |
| 27:BA:446:G:OP1   | 43:BU:3:ARG:NH1   | 2.48                     | 0.45              |
| 43:BU:42:ALA:C    | 43:BU:44:ASN:N    | 2.70                     | 0.45              |
| 1:CA:1223:C:H5    | 1:CA:1224:G:N7    | 2.15                     | 0.45              |
| 1:CA:1281:U:H5''  | 1:CA:1282:C:H5    | 1.82                     | 0.45              |
| 1:CA:152:A:H2'    | 1:CA:153:C:H5'    | 1.99                     | 0.45              |
| 1:CA:436:C:H2'    | 1:CA:437:U:C6     | 2.52                     | 0.45              |
| 1:CA:511:C:HO2'   | 1:CA:512:U:H6     | 1.62                     | 0.45              |
| 1:CA:525:C:H5''   | 12:CL:88:LYS:HZ3  | 1.81                     | 0.45              |
| 1:CA:883:C:N3     | 1:CA:884:U:C4     | 2.85                     | 0.45              |
| 3:CC:23:TYR:CD2   | 3:CC:24:ALA:N     | 2.85                     | 0.45              |
| 4:CD:22:LYS:HG3   | 4:CD:26:CYS:SG    | 2.56                     | 0.45              |
| 4:CD:79:PHE:O     | 4:CD:82:ALA:N     | 2.40                     | 0.45              |
| 6:CF:89:MET:SD    | 18:CR:76:LEU:HD11 | 2.57                     | 0.45              |
| 9:CI:18:PHE:HD1   | 9:CI:62:TYR:CD2   | 2.34                     | 0.45              |
| 9:CI:79:LEU:C     | 9:CI:79:LEU:HD13  | 2.36                     | 0.45              |
| 15:CO:2:PRO:HB2   | 15:CO:3:ILE:HD13  | 1.98                     | 0.45              |
| 17:CQ:12:SER:HB3  | 17:CQ:20:THR:OG1  | 2.17                     | 0.45              |
| 19:CS:62:ILE:CG2  | 19:CS:62:ILE:O    | 2.63                     | 0.45              |
| 23:CW:28:G:C2     | 23:CW:29:G:H1'    | 2.52                     | 0.45              |
| 49:D0:50:ASN:O    | 49:D0:51:VAL:HG23 | 2.16                     | 0.45              |
| 49:D0:7:LEU:HA    | 49:D0:7:LEU:HD23  | 1.70                     | 0.45              |
| 50:D1:16:ASN:HA   | 50:D1:38:SER:O    | 2.16                     | 0.45              |
| 51:D2:64:LEU:O    | 51:D2:64:LEU:HD23 | 2.17                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 58:D9:27:CYS:SG    | 58:D9:28:GLU:N    | 2.89                     | 0.45              |
| 27:DA:1296:G:H2'   | 27:DA:1297:C:C6   | 2.52                     | 0.45              |
| 27:DA:1323:U:OP1   | 45:DW:84:ARG:NE   | 2.50                     | 0.45              |
| 27:DA:1417:C:H2'   | 27:DA:1418:G:O4'  | 2.16                     | 0.45              |
| 27:DA:1549:C:O2    | 27:DA:1549:C:H2'  | 2.17                     | 0.45              |
| 27:DA:1380:G:O2'   | 27:DA:1569:A:N6   | 2.50                     | 0.45              |
| 27:DA:1700:A:C2'   | 27:DA:1701:A:O4'  | 2.64                     | 0.45              |
| 27:DA:1799:G:C5'   | 27:DA:1819:A:N6   | 2.77                     | 0.45              |
| 27:DA:1892:C:O2'   | 27:DA:1893:C:H5'  | 2.17                     | 0.45              |
| 27:DA:2201:C:H42   | 27:DA:2222:G:H1   | 1.64                     | 0.45              |
| 27:DA:2261:C:O4'   | 27:DA:2388:A:H1'  | 2.17                     | 0.45              |
| 27:DA:2391:G:H1    | 27:DA:2424:C:H2'  | 1.82                     | 0.45              |
| 27:DA:2069:G:N2    | 27:DA:2442:C:C2   | 2.81                     | 0.45              |
| 27:DA:254:G:H22    | 57:D8:8:LYS:NZ    | 2.15                     | 0.45              |
| 27:DA:292:C:C2'    | 27:DA:293:U:H5'   | 2.47                     | 0.45              |
| 27:DA:377:C:C4     | 27:DA:378:C:C5    | 3.05                     | 0.45              |
| 27:DA:468:G:N7     | 56:D7:39:ARG:NH2  | 2.58                     | 0.45              |
| 27:DA:667:U:H3'    | 27:DA:668:G:H5''  | 1.99                     | 0.45              |
| 27:DA:675:A:H2'    | 27:DA:676:A:H5'   | 1.99                     | 0.45              |
| 27:DA:815:C:OP1    | 44:DV:85:LYS:NZ   | 2.47                     | 0.45              |
| 27:DA:836:G:C5     | 27:DA:837:C:C4    | 3.05                     | 0.45              |
| 28:DB:43:C:C5      | 28:DB:45:A:N6     | 2.85                     | 0.45              |
| 30:DD:208:LYS:HG2  | 30:DD:211:ARG:HB3 | 1.98                     | 0.45              |
| 27:DA:1491:G:O4'   | 30:DD:99:ASP:OD2  | 2.34                     | 0.45              |
| 31:DE:196:VAL:O    | 31:DE:196:VAL:CG2 | 2.64                     | 0.45              |
| 31:DE:199:ARG:HB3  | 31:DE:200:GLU:OE2 | 2.16                     | 0.45              |
| 31:DE:49:LEU:N     | 31:DE:49:LEU:HD12 | 2.32                     | 0.45              |
| 32:DF:32:LEU:HD22  | 32:DF:112:MET:HE1 | 1.99                     | 0.45              |
| 32:DF:65:TRP:CH2   | 32:DF:75:HIS:HD2  | 2.34                     | 0.45              |
| 34:DH:102:ALA:HB1  | 34:DH:116:GLU:HA  | 1.99                     | 0.45              |
| 34:DH:26:VAL:O     | 34:DH:79:VAL:HG11 | 2.17                     | 0.45              |
| 37:DO:116:SER:C    | 37:DO:118:ALA:N   | 2.70                     | 0.45              |
| 37:DO:97:ARG:O     | 37:DO:98:VAL:CG1  | 2.61                     | 0.45              |
| 38:DP:6:LEU:HD12   | 38:DP:8:PRO:HG2   | 1.99                     | 0.45              |
| 39:DQ:134:ARG:HH12 | 48:DZ:118:GLU:CD  | 2.20                     | 0.45              |
| 40:DR:43:GLU:C     | 40:DR:45:ARG:H    | 2.20                     | 0.45              |
| 40:DR:83:ILE:O     | 40:DR:84:ALA:C    | 2.55                     | 0.45              |
| 42:DT:28:VAL:O     | 42:DT:29:ARG:CB   | 2.54                     | 0.45              |
| 42:DT:30:VAL:HG23  | 42:DT:31:SER:N    | 2.31                     | 0.45              |
| 45:DW:14:PRO:HG3   | 45:DW:101:SER:OG  | 2.16                     | 0.45              |
| 46:DX:64:LYS:HZ3   | 46:DX:73:ARG:CZ   | 2.28                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 47:DY:87:LYS:HG3   | 47:DY:88:LYS:H      | 1.81                     | 0.45              |
| 39:DQ:132:VAL:HB   | 48:DZ:80:ARG:HH22   | 1.81                     | 0.45              |
| 48:DZ:97:MET:H     | 48:DZ:124:LEU:CD1   | 2.30                     | 0.45              |
| 1:AA:1264:C:O2'    | 1:AA:1265:G:H5'     | 2.18                     | 0.44              |
| 1:AA:270:A:O2'     | 1:AA:271:C:H5'      | 2.16                     | 0.44              |
| 1:AA:393:A:O2'     | 1:AA:394:G:H5'      | 2.17                     | 0.44              |
| 1:AA:624:C:H4'     | 16:AP:10:GLY:HA2    | 1.99                     | 0.44              |
| 1:AA:63:C:N4       | 1:AA:105:G:C6       | 2.85                     | 0.44              |
| 1:AA:641:U:H4'     | 1:AA:642:A:OP1      | 2.17                     | 0.44              |
| 1:AA:592:G:C6      | 1:AA:648:A:N1       | 2.86                     | 0.44              |
| 1:AA:939:G:C2      | 1:AA:940:C:N3       | 2.85                     | 0.44              |
| 1:AA:952:U:C5      | 13:AM:104:ARG:NH2   | 2.83                     | 0.44              |
| 2:AB:132:LYS:HA    | 2:AB:135:GLN:HB2    | 1.98                     | 0.44              |
| 1:AA:1055:A:H1'    | 3:AC:156:ARG:NH1    | 2.31                     | 0.44              |
| 3:AC:16:ARG:CZ     | 3:AC:16:ARG:HB2     | 2.45                     | 0.44              |
| 5:AE:78:HIS:N      | 5:AE:78:HIS:ND1     | 2.65                     | 0.44              |
| 6:AF:75:LEU:C      | 6:AF:75:LEU:CD2     | 2.82                     | 0.44              |
| 8:AH:97:VAL:O      | 8:AH:99:GLU:N       | 2.49                     | 0.44              |
| 15:AO:24:SER:O     | 15:AO:28:GLN:NE2    | 2.34                     | 0.44              |
| 15:AO:63:ARG:O     | 15:AO:66:LEU:HB2    | 2.16                     | 0.44              |
| 16:AP:65:GLN:N     | 16:AP:65:GLN:OE1    | 2.50                     | 0.44              |
| 25:AY:57:A:H3'     | 25:AY:57:A:P        | 2.57                     | 0.44              |
| 55:B6:11:LEU:O     | 55:B6:23:THR:HA     | 2.17                     | 0.44              |
| 27:BA:1007:C:OP1   | 36:BN:37:LYS:NZ     | 2.46                     | 0.44              |
| 27:BA:1022:G:C6    | 27:BA:1141:U:C5     | 3.05                     | 0.44              |
| 27:BA:1141:U:H4'   | 27:BA:1142(A):A:O4' | 2.17                     | 0.44              |
| 27:BA:1230:C:H2'   | 27:BA:1231:G:H8     | 1.82                     | 0.44              |
| 27:BA:1359:A:H8    | 27:BA:1359:A:H5'    | 1.81                     | 0.44              |
| 27:BA:1419:A:H2'   | 27:BA:1421:G:N7     | 2.32                     | 0.44              |
| 27:BA:1495:A:H2'   | 27:BA:1496:A:N3     | 2.33                     | 0.44              |
| 27:BA:1499:C:C3'   | 27:BA:1500:G:H5'    | 2.47                     | 0.44              |
| 27:BA:1555:G:H2'   | 27:BA:1556:C:C6     | 2.51                     | 0.44              |
| 27:BA:1380:G:N2    | 27:BA:1570:A:H2     | 2.15                     | 0.44              |
| 27:BA:1787:A:O2'   | 27:BA:2589:A:H4'    | 2.17                     | 0.44              |
| 27:BA:1853:A:N3    | 27:BA:2233:U:O2'    | 2.48                     | 0.44              |
| 27:BA:363(A):A:H3' | 27:BA:363(B):G:H8   | 1.82                     | 0.44              |
| 27:BA:480:A:OP2    | 47:BY:46:LYS:NZ     | 2.48                     | 0.44              |
| 27:BA:699:A:C8     | 27:BA:700:G:C8      | 3.05                     | 0.44              |
| 27:BA:745:G:H2'    | 27:BA:746:A:H5'     | 1.99                     | 0.44              |
| 27:BA:992:C:C2'    | 27:BA:993:G:H5'     | 2.46                     | 0.44              |
| 29:BC:100:ILE:HG23 | 29:BC:131:LEU:O     | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BD:270:ILE:O   | 30:BD:271:ILE:CG2 | 2.60                     | 0.44              |
| 32:BF:113:ALA:HB1 | 32:BF:186:ILE:CG2 | 2.45                     | 0.44              |
| 34:BH:44:VAL:HG12 | 34:BH:45:VAL:HG23 | 1.98                     | 0.44              |
| 36:BN:3:THR:HG22  | 36:BN:4:TYR:H     | 1.82                     | 0.44              |
| 37:BO:57:VAL:O    | 37:BO:57:VAL:HG12 | 2.17                     | 0.44              |
| 39:BQ:69:PHE:C    | 39:BQ:69:PHE:CD2  | 2.90                     | 0.44              |
| 39:BQ:12:GLN:NE2  | 39:BQ:73:PRO:CD   | 2.80                     | 0.44              |
| 40:BR:87:TYR:CE1  | 40:BR:117:VAL:O   | 2.70                     | 0.44              |
| 41:BS:12:PHE:O    | 41:BS:14:VAL:HG23 | 2.18                     | 0.44              |
| 41:BS:24:LEU:HD12 | 41:BS:82:ILE:CG2  | 2.47                     | 0.44              |
| 46:BX:12:VAL:CG2  | 46:BX:13:LEU:N    | 2.75                     | 0.44              |
| 47:BY:83:THR:O    | 47:BY:84:ARG:HG3  | 2.17                     | 0.44              |
| 48:BZ:38:VAL:HG21 | 48:BZ:43:PHE:HB2  | 1.98                     | 0.44              |
| 48:BZ:55:VAL:HG12 | 48:BZ:56:ILE:N    | 2.31                     | 0.44              |
| 1:CA:1014:A:C2    | 1:CA:1219:U:H1'   | 2.52                     | 0.44              |
| 1:CA:945:G:C2     | 1:CA:1337:G:C2    | 3.05                     | 0.44              |
| 1:CA:1459:C:C2    | 1:CA:1460:A:C8    | 3.05                     | 0.44              |
| 1:CA:637:G:C2     | 1:CA:638:G:C5     | 3.06                     | 0.44              |
| 1:CA:667:G:O2'    | 1:CA:668:G:H5'    | 2.16                     | 0.44              |
| 2:CB:114:ARG:HH12 | 2:CB:118:LEU:HD21 | 1.82                     | 0.44              |
| 2:CB:139:LYS:HA   | 2:CB:139:LYS:HD3  | 1.77                     | 0.44              |
| 2:CB:89:GLY:O     | 2:CB:154:LEU:HD13 | 2.17                     | 0.44              |
| 2:CB:168:THR:O    | 2:CB:169:LYS:C    | 2.55                     | 0.44              |
| 2:CB:91:PRO:HG2   | 2:CB:155:LEU:CD2  | 2.47                     | 0.44              |
| 6:CF:6:VAL:HA     | 6:CF:90:VAL:HG13  | 1.99                     | 0.44              |
| 8:CH:104:ARG:NH2  | 8:CH:138:TRP:CH2  | 2.86                     | 0.44              |
| 8:CH:20:TYR:CE2   | 8:CH:75:ARG:HB3   | 2.53                     | 0.44              |
| 12:CL:29:PHE:O    | 12:CL:30:ARG:HB2  | 2.17                     | 0.44              |
| 17:CQ:77:VAL:O    | 17:CQ:78:GLU:CB   | 2.62                     | 0.44              |
| 19:CS:32:LYS:HB3  | 19:CS:57:HIS:NE2  | 2.32                     | 0.44              |
| 19:CS:45:VAL:C    | 19:CS:47:HIS:H    | 2.21                     | 0.44              |
| 20:CT:51:GLU:O    | 20:CT:52:ALA:C    | 2.54                     | 0.44              |
| 23:CW:37:U:O2'    | 23:CW:38:U:H5'    | 2.17                     | 0.44              |
| 23:CW:52:G:H1     | 23:CW:60:C:H42    | 1.65                     | 0.44              |
| 50:D1:49:VAL:O    | 50:D1:59:THR:HA   | 2.17                     | 0.44              |
| 27:DA:1021:A:C6   | 27:DA:1023:U:C4   | 3.05                     | 0.44              |
| 27:DA:1045:A:H4'  | 27:DA:1047:G:O4'  | 2.16                     | 0.44              |
| 27:DA:1042:G:C1'  | 27:DA:1114:G:N2   | 2.78                     | 0.44              |
| 27:DA:15:G:C4     | 27:DA:16:G:C8     | 3.05                     | 0.44              |
| 27:DA:574:C:C1'   | 27:DA:2055:C:H6   | 2.25                     | 0.44              |
| 27:DA:2236:C:H2'  | 27:DA:2237:G:H5'  | 1.98                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2250:G:C8    | 27:DA:2496:C:H5''  | 2.52                     | 0.44              |
| 27:DA:2406:U:O4    | 38:DP:70:GLN:HB3   | 2.17                     | 0.44              |
| 27:DA:2404:C:N4    | 27:DA:2414:G:O6    | 2.50                     | 0.44              |
| 27:DA:2552:U:H3    | 27:DA:2554:U:H5'   | 1.81                     | 0.44              |
| 27:DA:271(C):C:H2' | 27:DA:271(D):G:H8  | 1.81                     | 0.44              |
| 27:DA:45:C:H2'     | 27:DA:47:C:C6      | 2.52                     | 0.44              |
| 27:DA:27:G:H22     | 27:DA:512:G:H2'    | 1.77                     | 0.44              |
| 27:DA:571:A:H1'    | 27:DA:573:G:H8     | 1.77                     | 0.44              |
| 27:DA:630:G:N2     | 27:DA:634:C:C4     | 2.85                     | 0.44              |
| 27:DA:671:C:H41    | 38:DP:42:SER:HA    | 1.82                     | 0.44              |
| 27:DA:753:C:O2     | 27:DA:754:C:C6     | 2.70                     | 0.44              |
| 27:DA:864:G:C6     | 27:DA:865:C:C5     | 3.06                     | 0.44              |
| 27:DA:956:G:N2     | 27:DA:959:A:C3'    | 2.75                     | 0.44              |
| 28:DB:30:C:N3      | 28:DB:31:C:H1'     | 2.32                     | 0.44              |
| 29:DC:45:ALA:O     | 29:DC:46:LYS:CB    | 2.65                     | 0.44              |
| 30:DD:58:HIS:NE2   | 30:DD:59:LYS:O     | 2.50                     | 0.44              |
| 31:DE:19:ARG:O     | 31:DE:20:ALA:C     | 2.55                     | 0.44              |
| 27:DA:320:A:H2'    | 32:DF:136:THR:HG21 | 1.99                     | 0.44              |
| 33:DG:20:ILE:HG23  | 33:DG:25:TYR:HB2   | 1.99                     | 0.44              |
| 33:DG:98:ARG:HD3   | 33:DG:98:ARG:H     | 1.82                     | 0.44              |
| 33:DG:98:ARG:H     | 33:DG:98:ARG:CD    | 2.30                     | 0.44              |
| 34:DH:89:ILE:O     | 34:DH:90:LYS:C     | 2.55                     | 0.44              |
| 36:DN:66:LYS:O     | 36:DN:70:LYS:CB    | 2.64                     | 0.44              |
| 39:DQ:34:LEU:CD1   | 39:DQ:118:LEU:HD22 | 2.41                     | 0.44              |
| 39:DQ:43:THR:CG2   | 39:DQ:94:VAL:HG12  | 2.44                     | 0.44              |
| 41:DS:59:LYS:CE    | 41:DS:68:GLN:NE2   | 2.80                     | 0.44              |
| 41:DS:16:ASN:ND2   | 41:DS:92:TYR:CE1   | 2.85                     | 0.44              |
| 46:DX:5:TYR:HE2    | 51:D2:30:ARG:NE    | 2.14                     | 0.44              |
| 1:AA:1092:A:H5''   | 7:AG:4:ARG:NH2     | 2.31                     | 0.44              |
| 1:AA:1102:A:C5     | 1:AA:1103:C:C5     | 3.06                     | 0.44              |
| 1:AA:1142:G:C8     | 1:AA:1143:G:N7     | 2.86                     | 0.44              |
| 1:AA:230:G:C4'     | 16:AP:23:ASP:OD2   | 2.65                     | 0.44              |
| 1:AA:264:U:O2'     | 1:AA:265:G:H5'     | 2.18                     | 0.44              |
| 1:AA:28:G:O2'      | 1:AA:296:U:H5''    | 2.17                     | 0.44              |
| 1:AA:374:A:C4      | 1:AA:375:U:C5      | 3.04                     | 0.44              |
| 1:AA:407:G:H1      | 1:AA:435:C:H42     | 1.65                     | 0.44              |
| 1:AA:409:G:H2'     | 1:AA:410:G:H5'     | 1.98                     | 0.44              |
| 1:AA:423:G:O2'     | 1:AA:424:G:H5'     | 2.17                     | 0.44              |
| 1:AA:500:G:C6      | 1:AA:546:G:C2      | 3.05                     | 0.44              |
| 1:AA:568:G:N3      | 1:AA:568:G:H2'     | 2.32                     | 0.44              |
| 1:AA:895:G:H2'     | 1:AA:896:C:C6      | 2.52                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:92:TYR:O     | 2:AB:151:GLY:O     | 2.35                     | 0.44              |
| 2:AB:17:PHE:CD2   | 2:AB:17:PHE:O      | 2.70                     | 0.44              |
| 3:AC:112:SER:HB3  | 3:AC:115:LEU:CD1   | 2.36                     | 0.44              |
| 3:AC:182:ILE:HD11 | 3:AC:203:PHE:HD1   | 1.77                     | 0.44              |
| 3:AC:186:PHE:CD2  | 3:AC:186:PHE:C     | 2.90                     | 0.44              |
| 5:AE:20:GLN:O     | 5:AE:23:GLY:O      | 2.36                     | 0.44              |
| 8:AH:21:LYS:O     | 8:AH:22:GLU:C      | 2.55                     | 0.44              |
| 9:AI:42:ARG:O     | 9:AI:43:ALA:C      | 2.55                     | 0.44              |
| 10:AJ:88:LEU:HD11 | 10:AJ:90:LEU:CD1   | 2.48                     | 0.44              |
| 13:AM:48:LEU:O    | 13:AM:49:THR:O     | 2.36                     | 0.44              |
| 13:AM:80:ARG:C    | 13:AM:82:MET:N     | 2.71                     | 0.44              |
| 15:AO:58:MET:O    | 15:AO:61:GLY:N     | 2.51                     | 0.44              |
| 19:AS:61:TYR:C    | 19:AS:62:ILE:HG22  | 2.38                     | 0.44              |
| 19:AS:46:GLY:H    | 19:AS:62:ILE:HG23  | 1.81                     | 0.44              |
| 50:B1:53:VAL:CG1  | 50:B1:54:ALA:N     | 2.80                     | 0.44              |
| 27:BA:1007:C:C5   | 27:BA:1008:C:H2'   | 2.53                     | 0.44              |
| 27:BA:119:A:O2'   | 27:BA:120:U:P      | 2.75                     | 0.44              |
| 27:BA:1248:G:C3'  | 27:BA:1249:U:H5''  | 2.47                     | 0.44              |
| 27:BA:1579:A:H2'  | 27:BA:1580:A:H8    | 1.79                     | 0.44              |
| 27:BA:2173:A:O2'  | 27:BA:2174:C:C5'   | 2.59                     | 0.44              |
| 27:BA:2266:A:H5'  | 27:BA:2267:A:N7    | 2.32                     | 0.44              |
| 27:BA:2355:C:H2'  | 27:BA:2356:C:O4'   | 2.18                     | 0.44              |
| 27:BA:2516:G:C2'  | 27:BA:2517:C:C5'   | 2.85                     | 0.44              |
| 27:BA:2701:C:C3'  | 27:BA:2702:U:C5'   | 2.67                     | 0.44              |
| 27:BA:480:A:OP2   | 47:BY:46:LYS:HE3   | 2.17                     | 0.44              |
| 27:BA:571:A:OP2   | 27:BA:2030:A:N6    | 2.50                     | 0.44              |
| 29:BC:58:VAL:CG2  | 29:BC:166:ASP:H    | 2.30                     | 0.44              |
| 29:BC:41:VAL:HG23 | 29:BC:178:ALA:HB3  | 1.98                     | 0.44              |
| 32:BF:19:GLU:O    | 32:BF:20:LEU:HD12  | 2.17                     | 0.44              |
| 32:BF:60:SER:OG   | 32:BF:61:GLY:N     | 2.50                     | 0.44              |
| 33:BG:139:LEU:H   | 33:BG:139:LEU:HD23 | 1.82                     | 0.44              |
| 33:BG:7:LEU:HA    | 33:BG:10:LYS:HB2   | 2.00                     | 0.44              |
| 34:BH:29:PRO:O    | 34:BH:30:LYS:CD    | 2.65                     | 0.44              |
| 35:BI:37:VAL:HG12 | 35:BI:38:LEU:HD12  | 2.00                     | 0.44              |
| 35:BI:83:ALA:HB2  | 35:BI:88:ILE:HA    | 1.98                     | 0.44              |
| 36:BN:23:LEU:CD1  | 36:BN:99:LEU:HA    | 2.47                     | 0.44              |
| 37:BO:35:VAL:HA   | 37:BO:62:VAL:CG1   | 2.47                     | 0.44              |
| 37:BO:60:ALA:CB   | 37:BO:86:ILE:HA    | 2.47                     | 0.44              |
| 42:BT:19:LEU:CD1  | 42:BT:19:LEU:N     | 2.80                     | 0.44              |
| 42:BT:34:VAL:HA   | 42:BT:39:ARG:O     | 2.17                     | 0.44              |
| 42:BT:67:SER:C    | 42:BT:68:TYR:O     | 2.55                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:BW:97:LYS:HE3  | 45:BW:99:ARG:CZ   | 2.47                     | 0.44              |
| 47:BY:76:CYS:HB2  | 47:BY:96:ILE:HD11 | 1.99                     | 0.44              |
| 1:CA:1138:G:C2    | 1:CA:1140:C:C4    | 3.05                     | 0.44              |
| 1:CA:946:A:C2     | 1:CA:1236:A:C2    | 3.04                     | 0.44              |
| 1:CA:129(A):G:N2  | 1:CA:189(E):U:O2' | 2.51                     | 0.44              |
| 1:CA:1386:G:C2    | 1:CA:1387:G:C8    | 3.04                     | 0.44              |
| 1:CA:1513:A:C6    | 1:CA:1514:C:N4    | 2.85                     | 0.44              |
| 1:CA:658:G:H2'    | 1:CA:659:U:H6     | 1.81                     | 0.44              |
| 2:CB:132:LYS:HG2  | 2:CB:132:LYS:O    | 2.17                     | 0.44              |
| 4:CD:209:ARG:HG2  | 4:CD:209:ARG:OXT  | 2.17                     | 0.44              |
| 5:CE:63:ARG:C     | 5:CE:65:ASN:H     | 2.21                     | 0.44              |
| 12:CL:57:LEU:C    | 12:CL:59:SER:N    | 2.70                     | 0.44              |
| 1:CA:1225:A:H5'   | 13:CM:103:THR:OG1 | 2.16                     | 0.44              |
| 1:CA:982:U:C5'    | 14:CN:6:LEU:HD11  | 2.43                     | 0.44              |
| 15:CO:43:LEU:C    | 15:CO:45:VAL:N    | 2.69                     | 0.44              |
| 1:CA:275:G:H5'    | 17:CQ:14:LYS:HB3  | 1.99                     | 0.44              |
| 20:CT:91:LEU:C    | 20:CT:93:GLU:N    | 2.70                     | 0.44              |
| 21:CU:18:TYR:CD2  | 21:CU:22:ARG:HD3  | 2.52                     | 0.44              |
| 23:CW:8:U:O4      | 23:CW:13:A:H2'    | 2.17                     | 0.44              |
| 54:D5:31:VAL:CG1  | 54:D5:42:PRO:HB3  | 2.48                     | 0.44              |
| 54:D5:41:PRO:HA   | 54:D5:42:PRO:HD2  | 1.88                     | 0.44              |
| 55:D6:14:THR:C    | 55:D6:16:CYS:H    | 2.21                     | 0.44              |
| 57:D8:41:ILE:HG13 | 57:D8:41:ILE:H    | 1.58                     | 0.44              |
| 27:DA:1157:G:H2'  | 27:DA:1158:C:H6   | 1.74                     | 0.44              |
| 27:DA:1429:G:C2   | 27:DA:1430:C:C2   | 3.05                     | 0.44              |
| 27:DA:1566:A:C8   | 30:DD:214:TRP:CZ3 | 3.06                     | 0.44              |
| 27:DA:1765:C:O5'  | 27:DA:1765:C:H6   | 2.00                     | 0.44              |
| 27:DA:1827:C:H2'  | 27:DA:1828:G:O4'  | 2.17                     | 0.44              |
| 27:DA:1839:G:C8   | 27:DA:1927:A:H1'  | 2.51                     | 0.44              |
| 27:DA:1963:U:C2'  | 27:DA:1963:U:O2   | 2.65                     | 0.44              |
| 27:DA:1986:A:H2'  | 27:DA:1986:A:N3   | 2.32                     | 0.44              |
| 27:DA:2019:A:H5'' | 43:DU:27:LEU:HD12 | 1.98                     | 0.44              |
| 27:DA:2145:C:HO2' | 27:DA:2146:C:P    | 2.40                     | 0.44              |
| 27:DA:2290:G:C6   | 27:DA:2291:U:C4   | 3.05                     | 0.44              |
| 27:DA:2283:C:C2   | 27:DA:2389:G:C2   | 3.05                     | 0.44              |
| 27:DA:2587:A:N6   | 27:DA:2608:G:O2'  | 2.46                     | 0.44              |
| 27:DA:823:G:H2'   | 27:DA:824:A:C8    | 2.52                     | 0.44              |
| 27:DA:83:G:O2'    | 27:DA:84:A:C8     | 2.66                     | 0.44              |
| 30:DD:148:GLU:HB2 | 30:DD:151:LYS:HD2 | 1.98                     | 0.44              |
| 30:DD:77:ALA:HB2  | 30:DD:97:TYR:HE2  | 1.76                     | 0.44              |
| 31:DE:59:VAL:O    | 31:DE:60:ASN:CB   | 2.65                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DF:20:LEU:HB3  | 32:DF:23:ASP:CG    | 2.37                     | 0.44              |
| 33:DG:53:LEU:C    | 33:DG:55:LYS:N     | 2.68                     | 0.44              |
| 34:DH:85:LYS:O    | 34:DH:133:VAL:N    | 2.47                     | 0.44              |
| 35:DI:82:ARG:HG3  | 35:DI:82:ARG:NH1   | 2.31                     | 0.44              |
| 38:DP:21:ARG:CG   | 38:DP:29:LYS:HE3   | 2.47                     | 0.44              |
| 39:DQ:116:GLU:O   | 39:DQ:119:ARG:N    | 2.50                     | 0.44              |
| 39:DQ:58:PHE:CD1  | 39:DQ:58:PHE:O     | 2.71                     | 0.44              |
| 40:DR:38:VAL:HB   | 40:DR:39:PRO:CD    | 2.35                     | 0.44              |
| 41:DS:19:LYS:HB3  | 41:DS:20:ARG:NH1   | 2.33                     | 0.44              |
| 41:DS:49:VAL:HG21 | 41:DS:76:LYS:O     | 2.17                     | 0.44              |
| 43:DU:14:HIS:C    | 43:DU:16:LYS:N     | 2.70                     | 0.44              |
| 43:DU:49:HIS:O    | 43:DU:53:ARG:N     | 2.47                     | 0.44              |
| 43:DU:52:ARG:HD3  | 43:DU:55:ARG:HE    | 1.82                     | 0.44              |
| 43:DU:88:ILE:HG22 | 44:DV:47:VAL:O     | 2.17                     | 0.44              |
| 44:DV:66:ARG:O    | 44:DV:67:GLY:O     | 2.35                     | 0.44              |
| 44:DV:97:LYS:HD3  | 44:DV:97:LYS:HA    | 1.85                     | 0.44              |
| 45:DW:29:LEU:O    | 45:DW:33:ARG:HG3   | 2.18                     | 0.44              |
| 27:DA:751:A:O4'   | 45:DW:90:ARG:HD3   | 2.17                     | 0.44              |
| 48:DZ:43:PHE:C    | 48:DZ:43:PHE:CD1   | 2.91                     | 0.44              |
| 48:DZ:96:GLU:OE2  | 48:DZ:124:LEU:HD21 | 2.17                     | 0.44              |
| 1:AA:1054:C:P     | 1:AA:1197:G:OP2    | 2.75                     | 0.44              |
| 1:AA:588:G:C6     | 1:AA:753:A:C8      | 3.05                     | 0.44              |
| 1:AA:959:A:C2'    | 1:AA:960:U:H4'     | 2.46                     | 0.44              |
| 1:AA:978:A:H8     | 1:AA:978:A:H5''    | 1.82                     | 0.44              |
| 2:AB:127:ILE:O    | 2:AB:127:ILE:HG22  | 2.17                     | 0.44              |
| 2:AB:204:ASN:ND2  | 2:AB:206:ASP:N     | 2.65                     | 0.44              |
| 4:AD:13:ARG:O     | 4:AD:15:GLU:N      | 2.47                     | 0.44              |
| 4:AD:38:TYR:O     | 4:AD:39:PRO:O      | 2.35                     | 0.44              |
| 1:AA:1080:A:H5''  | 5:AE:16:THR:HG21   | 1.99                     | 0.44              |
| 1:AA:1346:A:H5'   | 9:AI:120:ARG:HH12  | 1.82                     | 0.44              |
| 9:AI:48:GLU:N     | 9:AI:49:PRO:CD     | 2.81                     | 0.44              |
| 10:AJ:38:ILE:HD11 | 10:AJ:71:LEU:HD23  | 2.00                     | 0.44              |
| 10:AJ:49:VAL:O    | 10:AJ:60:ARG:HB3   | 2.17                     | 0.44              |
| 11:AK:98:LEU:HA   | 11:AK:101:SER:HB3  | 1.98                     | 0.44              |
| 12:AL:37:VAL:HG11 | 12:AL:74:LEU:O     | 2.17                     | 0.44              |
| 15:AO:18:PHE:O    | 15:AO:19:PRO:C     | 2.55                     | 0.44              |
| 17:AQ:63:ARG:HH11 | 17:AQ:63:ARG:HB3   | 1.80                     | 0.44              |
| 23:AW:56:G:H2'    | 23:AW:57:A:H5'     | 1.99                     | 0.44              |
| 24:AX:29:G:H2'    | 24:AX:30:G:C8      | 2.47                     | 0.44              |
| 49:B0:17:GLN:O    | 49:B0:18:ALA:O     | 2.35                     | 0.44              |
| 49:B0:29:GLN:O    | 49:B0:67:VAL:HG23  | 2.18                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:B1:44:PRO:O     | 50:B1:46:LEU:HD13 | 2.17                     | 0.44              |
| 55:B6:19:ARG:H     | 55:B6:19:ARG:CD   | 2.21                     | 0.44              |
| 57:B8:63:PRO:HB2   | 57:B8:64:TYR:CD1  | 2.52                     | 0.44              |
| 27:BA:1013:C:C2'   | 27:BA:1014:U:H5'  | 2.48                     | 0.44              |
| 27:BA:102:G:OP1    | 27:BA:102:G:H4'   | 2.16                     | 0.44              |
| 27:BA:1440:G:H2'   | 27:BA:1441:G:O4'  | 2.18                     | 0.44              |
| 27:BA:1799:G:N1    | 27:BA:1819:A:N7   | 2.65                     | 0.44              |
| 27:BA:1924:C:H2'   | 27:BA:1925:C:H5'  | 1.99                     | 0.44              |
| 27:BA:528:A:H2     | 27:BA:2043:C:H5'  | 1.81                     | 0.44              |
| 27:BA:2302:G:C6    | 27:BA:2303:G:C5   | 3.05                     | 0.44              |
| 27:BA:237:C:O2'    | 27:BA:238:C:H5'   | 2.17                     | 0.44              |
| 27:BA:2481:G:HO2'  | 27:BA:2482:G:P    | 2.38                     | 0.44              |
| 27:BA:2611:U:H5'   | 27:BA:2611:U:C6   | 2.41                     | 0.44              |
| 27:BA:2654:A:C4'   | 27:BA:2655:G:OP1  | 2.62                     | 0.44              |
| 27:BA:26:G:H1'     | 27:BA:514:A:N6    | 2.32                     | 0.44              |
| 27:BA:271(L):U:H4' | 27:BA:271(M):G:C5 | 2.53                     | 0.44              |
| 27:BA:335:C:H5''   | 47:BY:73:ARG:CZ   | 2.48                     | 0.44              |
| 27:BA:36:G:H4'     | 27:BA:451:C:C2    | 2.51                     | 0.44              |
| 27:BA:481:G:O2'    | 27:BA:482:A:P     | 2.76                     | 0.44              |
| 27:BA:519:U:H6     | 27:BA:519:U:O5'   | 1.99                     | 0.44              |
| 27:BA:887:A:C2'    | 27:BA:888:C:H5''  | 2.48                     | 0.44              |
| 29:BC:90:GLY:O     | 29:BC:91:ALA:HB2  | 2.17                     | 0.44              |
| 30:BD:60:ARG:HG2   | 30:BD:61:LEU:H    | 1.83                     | 0.44              |
| 32:BF:51:THR:CG2   | 32:BF:92:PRO:HD2  | 2.46                     | 0.44              |
| 33:BG:72:ARG:HG2   | 33:BG:86:MET:O    | 2.17                     | 0.44              |
| 34:BH:85:LYS:CE    | 34:BH:141:VAL:O   | 2.65                     | 0.44              |
| 36:BN:82:LEU:HD12  | 36:BN:82:LEU:HA   | 1.73                     | 0.44              |
| 38:BP:9:ASN:O      | 38:BP:10:PRO:C    | 2.55                     | 0.44              |
| 39:BQ:114:ALA:O    | 39:BQ:116:GLU:N   | 2.50                     | 0.44              |
| 39:BQ:56:ARG:CG    | 39:BQ:56:ARG:HH11 | 2.26                     | 0.44              |
| 40:BR:27:SER:C     | 40:BR:34:ILE:HD11 | 2.37                     | 0.44              |
| 48:BZ:128:SER:C    | 48:BZ:130:ARG:H   | 2.19                     | 0.44              |
| 48:BZ:4:LEU:HD11   | 48:BZ:42:GLU:HB3  | 2.00                     | 0.44              |
| 48:BZ:8:TYR:OH     | 48:BZ:34:ARG:HG3  | 2.17                     | 0.44              |
| 1:CA:1105:A:C2     | 1:CA:1106:G:C5    | 3.05                     | 0.44              |
| 1:CA:1177:G:H22    | 1:CA:1181:G:H1    | 1.64                     | 0.44              |
| 1:CA:1054:C:H5     | 1:CA:1196:U:C6    | 2.34                     | 0.44              |
| 1:CA:1250:A:O2'    | 1:CA:1251:A:H5'   | 2.17                     | 0.44              |
| 1:CA:1278:U:H5''   | 1:CA:1279:A:H5'   | 2.00                     | 0.44              |
| 1:CA:1349:A:C2     | 1:CA:1350:A:C4    | 3.06                     | 0.44              |
| 1:CA:1324:A:C4'    | 1:CA:1362:C:H4'   | 2.46                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:CA:227:G:H2'     | 1:CA:228:A:C8       | 2.45                     | 0.44              |
| 1:CA:416:G:H2'     | 1:CA:417:C:C6       | 2.53                     | 0.44              |
| 1:CA:507:C:C2'     | 1:CA:508:C:H5       | 2.22                     | 0.44              |
| 1:CA:721:G:C4'     | 1:CA:722:A:O5'      | 2.42                     | 0.44              |
| 2:CB:124:SER:C     | 2:CB:126:GLU:H      | 2.21                     | 0.44              |
| 2:CB:127:ILE:O     | 2:CB:128:GLU:C      | 2.54                     | 0.44              |
| 2:CB:14:GLY:O      | 2:CB:15:VAL:CG1     | 2.54                     | 0.44              |
| 4:CD:185:PHE:CD2   | 4:CD:185:PHE:O      | 2.70                     | 0.44              |
| 5:CE:20:GLN:O      | 5:CE:21:ALA:C       | 2.55                     | 0.44              |
| 6:CF:1:MET:HE1     | 6:CF:68:PRO:HD3     | 1.99                     | 0.44              |
| 7:CG:15:ASP:CG     | 7:CG:16:LEU:H       | 2.21                     | 0.44              |
| 8:CH:48:TYR:CD1    | 8:CH:48:TYR:C       | 2.90                     | 0.44              |
| 8:CH:9:MET:HB2     | 8:CH:26:VAL:CG2     | 2.48                     | 0.44              |
| 9:CI:25:LYS:HG3    | 9:CI:25:LYS:O       | 2.16                     | 0.44              |
| 9:CI:8:GLY:HA3     | 9:CI:76:ALA:O       | 2.18                     | 0.44              |
| 12:CL:5:ASN:O      | 12:CL:8:VAL:CB      | 2.65                     | 0.44              |
| 20:CT:94:ALA:O     | 20:CT:95:ALA:HB3    | 2.17                     | 0.44              |
| 50:D1:19:GLN:O     | 50:D1:35:THR:N      | 2.47                     | 0.44              |
| 51:D2:7:ARG:O      | 51:D2:11:GLU:HG3    | 2.17                     | 0.44              |
| 52:D3:47:VAL:HA    | 52:D3:50:VAL:CG2    | 2.47                     | 0.44              |
| 27:DA:2815:C:O2'   | 54:D5:43:HIS:CD2    | 2.71                     | 0.44              |
| 27:DA:125:G:N2     | 56:D7:48:LYS:HE3    | 2.18                     | 0.44              |
| 58:D9:25:VAL:HG21  | 58:D9:34:GLN:OE1    | 2.17                     | 0.44              |
| 27:DA:1114:G:C3'   | 27:DA:1115:G:H5''   | 2.47                     | 0.44              |
| 27:DA:1322:A:C8    | 27:DA:1323:U:H5     | 2.35                     | 0.44              |
| 27:DA:1432:C:C4    | 27:DA:1433:U:C5     | 3.05                     | 0.44              |
| 27:DA:1450(A):C:H6 | 27:DA:1450(A):C:O5' | 2.00                     | 0.44              |
| 27:DA:1485:G:H8    | 27:DA:1485:G:H5'    | 1.83                     | 0.44              |
| 27:DA:154:G:C5     | 27:DA:154(A):C:N3   | 2.86                     | 0.44              |
| 27:DA:1705:G:H2'   | 27:DA:1706:U:O4'    | 2.18                     | 0.44              |
| 27:DA:1852:C:H6    | 27:DA:1852:C:H3'    | 1.83                     | 0.44              |
| 27:DA:1896:G:C6    | 27:DA:1897:G:N7     | 2.86                     | 0.44              |
| 27:DA:2089:U:H6    | 27:DA:2089:U:H5''   | 1.83                     | 0.44              |
| 27:DA:2187:G:C5    | 27:DA:2188:C:C4     | 3.06                     | 0.44              |
| 27:DA:2297:C:H2'   | 27:DA:2298:A:C8     | 2.52                     | 0.44              |
| 27:DA:2437:U:H2'   | 27:DA:2438:U:C6     | 2.52                     | 0.44              |
| 27:DA:2462:U:H2'   | 27:DA:2463:C:O4'    | 2.17                     | 0.44              |
| 27:DA:2534:A:N6    | 27:DA:2535:G:C5     | 2.85                     | 0.44              |
| 27:DA:271(J):C:C3' | 27:DA:271(K):U:H5'' | 2.47                     | 0.44              |
| 27:DA:310:A:C6     | 27:DA:330:A:C6      | 3.05                     | 0.44              |
| 27:DA:376:C:H2'    | 27:DA:377:C:H6      | 1.81                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:386:G:O2'    | 27:DA:387:U:OP1    | 2.31                     | 0.44              |
| 27:DA:677:A:H2'    | 27:DA:678:C:C6     | 2.52                     | 0.44              |
| 27:DA:777:A:C2'    | 27:DA:778:G:H5'    | 2.48                     | 0.44              |
| 28:DB:30:C:C2      | 28:DB:31:C:H1'     | 2.53                     | 0.44              |
| 29:DC:39:GLU:HG2   | 29:DC:180:PHE:CB   | 2.48                     | 0.44              |
| 29:DC:189:ILE:C    | 29:DC:191:ALA:N    | 2.71                     | 0.44              |
| 30:DD:157:ARG:HG3  | 30:DD:157:ARG:HH11 | 1.82                     | 0.44              |
| 30:DD:158:ALA:HB3  | 30:DD:161:THR:CG2  | 2.48                     | 0.44              |
| 31:DE:13:ARG:HD2   | 31:DE:20:ALA:HB1   | 1.99                     | 0.44              |
| 31:DE:110:GLY:HA2  | 31:DE:161:GLY:HA3  | 1.98                     | 0.44              |
| 31:DE:26:ILE:CB    | 31:DE:182:LEU:HB3  | 2.42                     | 0.44              |
| 32:DF:65:TRP:O     | 32:DF:67:GLN:N     | 2.51                     | 0.44              |
| 34:DH:139:GLN:HG3  | 34:DH:140:LYS:H    | 1.83                     | 0.44              |
| 34:DH:54:ARG:NH2   | 34:DH:57:ASP:OD1   | 2.50                     | 0.44              |
| 35:DI:39:ALA:O     | 35:DI:40:THR:O     | 2.36                     | 0.44              |
| 36:DN:11:PRO:O     | 36:DN:13:TRP:N     | 2.50                     | 0.44              |
| 36:DN:131:GLN:HE22 | 36:DN:134:ARG:HD2  | 1.82                     | 0.44              |
| 37:DO:71:ARG:NE    | 37:DO:105:GLU:OE2  | 2.39                     | 0.44              |
| 38:DP:79:ARG:NH2   | 38:DP:109:GLY:CA   | 2.80                     | 0.44              |
| 27:DA:587:C:C5     | 38:DP:33:ARG:HD3   | 2.51                     | 0.44              |
| 39:DQ:40:ALA:HB3   | 39:DQ:127:ILE:HD13 | 1.99                     | 0.44              |
| 39:DQ:70:PRO:HA    | 39:DQ:94:VAL:O     | 2.18                     | 0.44              |
| 40:DR:30:THR:O     | 40:DR:30:THR:CG2   | 2.63                     | 0.44              |
| 42:DT:74:ARG:HD3   | 42:DT:76:PHE:CZ    | 2.51                     | 0.44              |
| 46:DX:72:LYS:N     | 46:DX:72:LYS:CD    | 2.81                     | 0.44              |
| 48:DZ:162:LEU:H    | 48:DZ:162:LEU:HD12 | 1.83                     | 0.44              |
| 1:AA:1400:C:C4     | 24:AX:34:C:C2      | 3.06                     | 0.44              |
| 1:AA:200:G:N2      | 1:AA:218:C:N3      | 2.65                     | 0.44              |
| 1:AA:225:C:H2'     | 1:AA:226:G:H8      | 1.83                     | 0.44              |
| 1:AA:232:G:H2'     | 1:AA:233:C:C6      | 2.49                     | 0.44              |
| 1:AA:384:G:H2'     | 1:AA:385:C:C6      | 2.53                     | 0.44              |
| 1:AA:52:G:O2'      | 1:AA:53:A:O5'      | 2.36                     | 0.44              |
| 1:AA:640:A:N3      | 8:AH:115:SER:HB2   | 2.32                     | 0.44              |
| 1:AA:667:G:N2      | 1:AA:740:U:H1'     | 2.32                     | 0.44              |
| 1:AA:956:U:O2'     | 1:AA:957:U:H5'     | 2.18                     | 0.44              |
| 2:AB:196:LEU:HG    | 2:AB:196:LEU:H     | 1.41                     | 0.44              |
| 2:AB:224:GLN:HE21  | 2:AB:229:VAL:CG2   | 2.30                     | 0.44              |
| 3:AC:57:ILE:HA     | 3:AC:65:ALA:HB3    | 1.98                     | 0.44              |
| 3:AC:82:GLU:O      | 3:AC:86:VAL:HG13   | 2.16                     | 0.44              |
| 8:AH:74:PRO:CG     | 8:AH:75:ARG:N      | 2.80                     | 0.44              |
| 9:AI:19:LEU:HB3    | 9:AI:59:PHE:HD2    | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:528:C:H41    | 12:AL:46:ASN:ND2  | 2.14                     | 0.44              |
| 1:AA:1226:C:O2'   | 13:AM:103:THR:O   | 2.24                     | 0.44              |
| 13:AM:4:ILE:CG2   | 13:AM:5:ALA:N     | 2.79                     | 0.44              |
| 14:AN:9:LYS:HA    | 14:AN:12:ARG:NH1  | 2.32                     | 0.44              |
| 18:AR:33:ASP:C    | 18:AR:33:ASP:OD2  | 2.55                     | 0.44              |
| 20:AT:30:LYS:HD3  | 20:AT:30:LYS:C    | 2.38                     | 0.44              |
| 20:AT:28:ALA:C    | 20:AT:30:LYS:N    | 2.71                     | 0.44              |
| 23:AW:23:G:H2'    | 23:AW:24:C:H6     | 1.81                     | 0.44              |
| 49:B0:24:LYS:O    | 49:B0:25:ARG:HD3  | 2.18                     | 0.44              |
| 49:B0:35:ASN:O    | 49:B0:60:PHE:HB2  | 2.16                     | 0.44              |
| 50:B1:46:LEU:H    | 50:B1:46:LEU:HD22 | 1.79                     | 0.44              |
| 50:B1:53:VAL:O    | 50:B1:54:ALA:C    | 2.55                     | 0.44              |
| 55:B6:15:GLU:OE1  | 55:B6:41:PRO:CB   | 2.66                     | 0.44              |
| 57:B8:41:ILE:HG13 | 57:B8:41:ILE:H    | 1.34                     | 0.44              |
| 27:BA:1140:C:P    | 36:BN:66:LYS:NZ   | 2.90                     | 0.44              |
| 27:BA:1286:A:C2   | 27:BA:1289:C:C6   | 3.05                     | 0.44              |
| 27:BA:1391:U:O2   | 27:BA:1393:A:H8   | 1.99                     | 0.44              |
| 27:BA:1408:C:O2   | 27:BA:1408:C:H2'  | 2.16                     | 0.44              |
| 27:BA:149:A:C2    | 27:BA:150:C:C2    | 3.05                     | 0.44              |
| 27:BA:1689:A:O2'  | 27:BA:1690:A:H5'  | 2.17                     | 0.44              |
| 27:BA:1695:G:N2   | 27:BA:1696:G:N7   | 2.65                     | 0.44              |
| 27:BA:1739:U:O2'  | 27:BA:1740:G:C5'  | 2.63                     | 0.44              |
| 27:BA:758:C:O2    | 27:BA:1981:A:H2   | 2.00                     | 0.44              |
| 27:BA:1991:U:C2'  | 27:BA:1992:G:H5'' | 2.47                     | 0.44              |
| 27:BA:2121:G:H2'  | 27:BA:2122:U:O4'  | 2.17                     | 0.44              |
| 27:BA:2174:C:O2'  | 27:BA:2175:C:C6   | 2.71                     | 0.44              |
| 27:BA:2203:U:O2   | 27:BA:2221:G:C2   | 2.70                     | 0.44              |
| 27:BA:2256:G:N2   | 27:BA:2275:C:C4   | 2.85                     | 0.44              |
| 27:BA:2534:A:C2   | 27:BA:2535:G:H1'  | 2.53                     | 0.44              |
| 27:BA:258:G:C4    | 27:BA:259:G:C8    | 3.06                     | 0.44              |
| 27:BA:2760:C:H6   | 27:BA:2760:C:O5'  | 2.01                     | 0.44              |
| 27:BA:2895:U:H5   | 27:BA:2896:C:N3   | 2.16                     | 0.44              |
| 27:BA:374:A:H61   | 27:BA:400:G:C2'   | 2.31                     | 0.44              |
| 27:BA:391:G:C8    | 27:BA:391:G:H5''  | 2.53                     | 0.44              |
| 27:BA:615:G:H2'   | 27:BA:616:G:O4'   | 2.17                     | 0.44              |
| 27:BA:662:G:OP1   | 38:BP:18:ARG:NH1  | 2.50                     | 0.44              |
| 27:BA:692:C:N3    | 27:BA:771:G:C2    | 2.86                     | 0.44              |
| 28:BB:20:C:C2'    | 28:BB:21:G:H5'    | 2.47                     | 0.44              |
| 31:BE:33:VAL:HG22 | 31:BE:33:VAL:O    | 2.17                     | 0.44              |
| 32:BF:41:LEU:CD1  | 32:BF:184:TYR:HE1 | 2.22                     | 0.44              |
| 32:BF:2:LYS:HG2   | 32:BF:25:PRO:CG   | 2.47                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:3:ARG:HH21   | 33:BG:139:LEU:HD11 | 1.83                     | 0.44              |
| 33:BG:119:GLY:HA3  | 33:BG:181:ARG:HB2  | 1.99                     | 0.44              |
| 33:BG:77:ILE:O     | 33:BG:77:ILE:HG22  | 2.17                     | 0.44              |
| 34:BH:121:ILE:HG23 | 34:BH:133:VAL:HG12 | 1.99                     | 0.44              |
| 35:BI:133:HIS:O    | 35:BI:135:GLU:N    | 2.51                     | 0.44              |
| 36:BN:121:LYS:HB3  | 36:BN:123:TYR:CE1  | 2.48                     | 0.44              |
| 36:BN:73:THR:HA    | 36:BN:83:LYS:O     | 2.18                     | 0.44              |
| 38:BP:99:LEU:HA    | 38:BP:102:ARG:NH1  | 2.32                     | 0.44              |
| 38:BP:106:LEU:O    | 38:BP:107:LYS:CG   | 2.65                     | 0.44              |
| 41:BS:54:LEU:HD13  | 41:BS:58:LEU:HB2   | 1.98                     | 0.44              |
| 41:BS:88:ASP:CG    | 41:BS:89:ARG:H     | 2.18                     | 0.44              |
| 42:BT:133:GLU:OE2  | 42:BT:137:LYS:HB2  | 2.17                     | 0.44              |
| 42:BT:22:PHE:CD2   | 42:BT:22:PHE:N     | 2.86                     | 0.44              |
| 42:BT:48:ILE:O     | 42:BT:50:ILE:CD1   | 2.66                     | 0.44              |
| 46:BX:11:PRO:HA    | 46:BX:28:PHE:HA    | 1.99                     | 0.44              |
| 48:BZ:142:GLY:O    | 48:BZ:143:LEU:HD22 | 2.17                     | 0.44              |
| 48:BZ:150:HIS:HB2  | 48:BZ:167:GLU:O    | 2.17                     | 0.44              |
| 1:CA:999:C:C2'     | 1:CA:1000:U:H5'    | 2.47                     | 0.44              |
| 1:CA:1004:A:H5'    | 1:CA:1025:U:H3     | 1.82                     | 0.44              |
| 1:CA:122:G:H2'     | 1:CA:123:C:O4'     | 2.18                     | 0.44              |
| 1:CA:806:C:H2'     | 1:CA:807:A:H8      | 1.82                     | 0.44              |
| 1:CA:979:C:C3'     | 1:CA:980:C:C5'     | 2.87                     | 0.44              |
| 2:CB:168:THR:O     | 2:CB:170:GLU:N     | 2.50                     | 0.44              |
| 4:CD:122:ARG:HA    | 4:CD:134:ASP:O     | 2.18                     | 0.44              |
| 4:CD:175:SER:HB3   | 4:CD:186:LEU:HD11  | 1.99                     | 0.44              |
| 4:CD:166:LYS:HG3   | 4:CD:178:VAL:HG11  | 1.99                     | 0.44              |
| 5:CE:147:ASP:O     | 5:CE:151:LEU:HG    | 2.18                     | 0.44              |
| 8:CH:44:PHE:HD1    | 8:CH:79:VAL:HG12   | 1.83                     | 0.44              |
| 11:CK:12:ARG:HG2   | 11:CK:13:GLN:N     | 2.32                     | 0.44              |
| 15:CO:33:THR:HG23  | 15:CO:63:ARG:NH1   | 2.32                     | 0.44              |
| 1:CA:742:G:P       | 15:CO:35:ARG:NH2   | 2.90                     | 0.44              |
| 25:CY:45:U:H5''    | 25:CY:46:U:OP1     | 2.18                     | 0.44              |
| 25:CY:71:A:O2'     | 25:CY:72:G:H5'     | 2.17                     | 0.44              |
| 25:CY:7:A:N6       | 25:CY:48:C:C5      | 2.85                     | 0.44              |
| 12:CL:41:THR:HG21  | 26:CZ:6:5OH:OS     | 2.18                     | 0.44              |
| 49:D0:47:PRO:HA    | 49:D0:51:VAL:HG12  | 1.98                     | 0.44              |
| 50:D1:40:ARG:HD3   | 50:D1:40:ARG:O     | 2.17                     | 0.44              |
| 50:D1:46:LEU:HA    | 50:D1:63:ALA:HA    | 1.98                     | 0.44              |
| 57:D8:29:LYS:HE2   | 57:D8:44:LYS:HB3   | 1.99                     | 0.44              |
| 27:DA:1429:G:N2    | 27:DA:1430:C:C2    | 2.85                     | 0.44              |
| 27:DA:1505:C:H2'   | 27:DA:1506:C:O5'   | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1624:G:H2'   | 27:DA:1625:C:H6    | 1.83                     | 0.44              |
| 27:DA:1679:U:H2'   | 27:DA:1680:U:O4'   | 2.17                     | 0.44              |
| 27:DA:1771:C:O2'   | 27:DA:1786:A:H8    | 2.01                     | 0.44              |
| 27:DA:1907:G:C2'   | 27:DA:1908:C:H5'   | 2.48                     | 0.44              |
| 27:DA:1932:A:H2'   | 27:DA:1933:G:C5'   | 2.47                     | 0.44              |
| 27:DA:1970:A:H4'   | 27:DA:1971:A:OP1   | 2.16                     | 0.44              |
| 27:DA:2162:G:C2    | 27:DA:2163:C:C2    | 3.05                     | 0.44              |
| 27:DA:2220:G:N2    | 27:DA:2221:G:H1'   | 2.33                     | 0.44              |
| 27:DA:2315:G:H2'   | 27:DA:2316:C:H6    | 1.82                     | 0.44              |
| 27:DA:2355:C:C1'   | 49:D0:36:ILE:HD11  | 2.48                     | 0.44              |
| 27:DA:2423:U:C2    | 27:DA:2425:A:C2    | 3.05                     | 0.44              |
| 27:DA:2426:A:H3'   | 27:DA:2427:C:H5'   | 1.97                     | 0.44              |
| 27:DA:245:G:H2'    | 27:DA:246:C:H6     | 1.82                     | 0.44              |
| 27:DA:2846:G:H2'   | 27:DA:2847:U:C6    | 2.52                     | 0.44              |
| 27:DA:313:C:O2'    | 27:DA:314:A:O4'    | 2.36                     | 0.44              |
| 27:DA:477:A:O2'    | 27:DA:478:A:O4'    | 2.34                     | 0.44              |
| 27:DA:621:A:H3'    | 27:DA:622:G:H8     | 1.82                     | 0.44              |
| 27:DA:660:G:C2'    | 27:DA:661:C:H5'    | 2.48                     | 0.44              |
| 27:DA:907:U:H6     | 27:DA:907:U:H5'    | 1.82                     | 0.44              |
| 27:DA:962:G:H2'    | 27:DA:963:U:H6     | 1.82                     | 0.44              |
| 28:DB:27:C:H6      | 28:DB:27:C:C5'     | 2.30                     | 0.44              |
| 28:DB:54:G:H21     | 33:DG:29:TRP:HE1   | 1.65                     | 0.44              |
| 31:DE:170:LEU:HD23 | 31:DE:185:LYS:O    | 2.18                     | 0.44              |
| 32:DF:8:GLN:O      | 32:DF:9:ILE:C      | 2.56                     | 0.44              |
| 34:DH:111:HIS:HA   | 34:DH:112:PRO:HD2  | 1.78                     | 0.44              |
| 34:DH:97:ARG:HB3   | 34:DH:98:LEU:H     | 1.54                     | 0.44              |
| 35:DI:77:LEU:HD12  | 35:DI:101:LEU:HD22 | 1.98                     | 0.44              |
| 36:DN:97:ARG:O     | 36:DN:100:GLU:N    | 2.50                     | 0.44              |
| 36:DN:128:HIS:ND1  | 36:DN:128:HIS:N    | 2.65                     | 0.44              |
| 36:DN:12:ARG:O     | 36:DN:13:TRP:C     | 2.54                     | 0.44              |
| 39:DQ:58:PHE:HB3   | 39:DQ:113:GLN:NE2  | 2.31                     | 0.44              |
| 42:DT:27:THR:OG1   | 42:DT:28:VAL:N     | 2.44                     | 0.44              |
| 43:DU:66:ASN:ND2   | 43:DU:70:ARG:HE    | 2.16                     | 0.44              |
| 46:DX:47:PHE:O     | 46:DX:49:VAL:HG13  | 2.17                     | 0.44              |
| 47:DY:68:HIS:HB3   | 47:DY:71:LYS:CG    | 2.47                     | 0.44              |
| 1:AA:1014:A:H2'    | 1:AA:1015:A:C8     | 2.53                     | 0.44              |
| 1:AA:1316:G:H1'    | 1:AA:1360:A:H2     | 1.82                     | 0.44              |
| 1:AA:1380:U:O2'    | 1:AA:1381:U:OP2    | 2.33                     | 0.44              |
| 1:AA:316:G:H2'     | 1:AA:317:G:H8      | 1.83                     | 0.44              |
| 1:AA:322:C:H2'     | 1:AA:323:U:C6      | 2.36                     | 0.44              |
| 1:AA:43:C:H2'      | 1:AA:44:G:O5'      | 2.18                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:580:U:C2'    | 1:AA:581:G:O4'     | 2.60                     | 0.44              |
| 1:AA:599:C:H4'    | 8:AH:130:GLY:C     | 2.37                     | 0.44              |
| 1:AA:742:G:O2'    | 1:AA:743:U:H5'     | 2.17                     | 0.44              |
| 1:AA:992:U:H3     | 1:AA:1044:A:N6     | 2.08                     | 0.44              |
| 3:AC:114:PRO:HG3  | 3:AC:185:GLY:CA    | 2.45                     | 0.44              |
| 3:AC:63:ASN:OD1   | 3:AC:63:ASN:N      | 2.50                     | 0.44              |
| 4:AD:193:ASP:C    | 4:AD:194:LEU:HD22  | 2.38                     | 0.44              |
| 5:AE:33:VAL:HG21  | 5:AE:109:ILE:CD1   | 2.47                     | 0.44              |
| 8:AH:54:ASP:HB2   | 8:AH:56:LYS:CE     | 2.45                     | 0.44              |
| 10:AJ:34:VAL:HG22 | 10:AJ:74:ILE:HG22  | 1.99                     | 0.44              |
| 13:AM:11:ARG:HB3  | 13:AM:12:ASN:CG    | 2.37                     | 0.44              |
| 1:AA:392:G:H5'    | 16:AP:13:HIS:CE1   | 2.52                     | 0.44              |
| 1:AA:277:C:OP1    | 17:AQ:41:LYS:HE3   | 2.18                     | 0.44              |
| 19:AS:18:LYS:HD2  | 19:AS:22:LEU:HD21  | 1.99                     | 0.44              |
| 19:AS:39:THR:HG23 | 19:AS:70:LYS:HE2   | 1.98                     | 0.44              |
| 46:BX:9:LEU:CA    | 51:B2:36:ARG:HH21  | 2.16                     | 0.44              |
| 55:B6:48:VAL:C    | 55:B6:49:HIS:ND1   | 2.71                     | 0.44              |
| 58:B9:19:ARG:HG3  | 58:B9:24:TYR:HE1   | 1.81                     | 0.44              |
| 27:BA:1300:U:C2'  | 27:BA:1301:A:OP2   | 2.66                     | 0.44              |
| 27:BA:1357:U:H2'  | 27:BA:1358:G:C8    | 2.52                     | 0.44              |
| 27:BA:1464:C:O2'  | 27:BA:1528:A:C8    | 2.70                     | 0.44              |
| 27:BA:176:G:H2'   | 27:BA:177:G:O4'    | 2.17                     | 0.44              |
| 27:BA:2078:C:H2'  | 27:BA:2079:U:H6    | 1.83                     | 0.44              |
| 27:BA:2119:A:O2'  | 27:BA:2120:G:H5''  | 2.17                     | 0.44              |
| 27:BA:2151:G:O2'  | 27:BA:2152:G:H5'   | 2.18                     | 0.44              |
| 27:BA:2553:G:H3'  | 27:BA:2554:U:C5'   | 2.44                     | 0.44              |
| 27:BA:270:A:O2'   | 27:BA:271:A:H5'    | 2.18                     | 0.44              |
| 27:BA:2778:A:C4'  | 27:BA:2779:U:OP2   | 2.64                     | 0.44              |
| 27:BA:491:G:C2'   | 27:BA:492:A:O5'    | 2.65                     | 0.44              |
| 27:BA:528:A:C2    | 27:BA:2043:C:H5'   | 2.53                     | 0.44              |
| 27:BA:608:A:C2    | 27:BA:621:A:C4     | 3.05                     | 0.44              |
| 27:BA:754:C:C2    | 27:BA:755:C:C5     | 3.05                     | 0.44              |
| 27:BA:828:U:H4'   | 27:BA:831:G:C6     | 2.52                     | 0.44              |
| 27:BA:845:G:C8    | 27:BA:845:G:OP2    | 2.71                     | 0.44              |
| 30:BD:268:ARG:HB3 | 30:BD:268:ARG:NH1  | 2.33                     | 0.44              |
| 31:BE:188:VAL:O   | 31:BE:188:VAL:HG13 | 2.16                     | 0.44              |
| 32:BF:18:ARG:CG   | 32:BF:199:TRP:HZ3  | 2.29                     | 0.44              |
| 24:AX:56:C:H1'    | 33:BG:76:SER:HB3   | 2.00                     | 0.44              |
| 27:BA:2748:A:OP1  | 34:BH:70:THR:HG21  | 2.17                     | 0.44              |
| 36:BN:35:ARG:O    | 36:BN:37:LYS:N     | 2.50                     | 0.44              |
| 38:BP:136:GLU:O   | 38:BP:139:LYS:HB3  | 2.17                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BS:89:ARG:HB3   | 41:BS:92:TYR:HB3  | 2.00                     | 0.44              |
| 47:BY:38:ILE:O     | 47:BY:39:VAL:CB   | 2.65                     | 0.44              |
| 48:BZ:126:LYS:HD3  | 48:BZ:161:GLU:OE1 | 2.18                     | 0.44              |
| 48:BZ:24:PRO:O     | 48:BZ:84:HIS:HA   | 2.17                     | 0.44              |
| 1:CA:1001(A):G:O2' | 1:CA:1002:G:H5'   | 2.18                     | 0.44              |
| 1:CA:1138:G:N2     | 1:CA:1140:C:N4    | 2.65                     | 0.44              |
| 1:CA:1190:G:OP1    | 3:CC:5:ILE:HG13   | 2.17                     | 0.44              |
| 1:CA:1304:G:N2     | 1:CA:1332:A:N7    | 2.65                     | 0.44              |
| 1:CA:1305:G:O2'    | 1:CA:1306:A:OP2   | 2.29                     | 0.44              |
| 1:CA:135:C:H2'     | 1:CA:136:C:C5'    | 2.45                     | 0.44              |
| 1:CA:324:G:N2      | 1:CA:327:A:C8     | 2.86                     | 0.44              |
| 1:CA:450:G:H2'     | 1:CA:451:A:OP1    | 2.17                     | 0.44              |
| 1:CA:648:A:C6      | 1:CA:649:G:C6     | 3.06                     | 0.44              |
| 1:CA:926:G:H8      | 1:CA:926:G:O5'    | 2.01                     | 0.44              |
| 1:CA:962:C:H2'     | 1:CA:963:G:C8     | 2.52                     | 0.44              |
| 1:CA:980:C:C2'     | 1:CA:980:C:O2     | 2.64                     | 0.44              |
| 2:CB:217:ARG:O     | 2:CB:221:LEU:HD23 | 2.18                     | 0.44              |
| 2:CB:39:ILE:HG22   | 2:CB:40:HIS:N     | 2.32                     | 0.44              |
| 3:CC:76:VAL:HG21   | 3:CC:103:VAL:HG11 | 1.98                     | 0.44              |
| 5:CE:67:VAL:HG22   | 5:CE:68:GLU:N     | 2.31                     | 0.44              |
| 7:CG:24:THR:O      | 7:CG:28:ASN:ND2   | 2.46                     | 0.44              |
| 1:CA:1149:C:OP1    | 9:CI:14:VAL:HG21  | 2.16                     | 0.44              |
| 9:CI:27:THR:HG22   | 9:CI:28:VAL:N     | 2.33                     | 0.44              |
| 9:CI:93:ARG:HD2    | 9:CI:93:ARG:HA    | 1.85                     | 0.44              |
| 10:CJ:9:ARG:O      | 10:CJ:94:VAL:HG13 | 2.17                     | 0.44              |
| 13:CM:81:LEU:HB3   | 13:CM:89:GLY:CA   | 2.47                     | 0.44              |
| 14:CN:39:LEU:HD13  | 14:CN:44:LEU:HA   | 1.99                     | 0.44              |
| 18:CR:33:ASP:HB3   | 18:CR:36:ASN:HD21 | 1.81                     | 0.44              |
| 20:CT:33:ILE:HD12  | 20:CT:63:ILE:HG12 | 1.99                     | 0.44              |
| 23:CW:44:A:H2'     | 23:CW:46:U:H6     | 1.82                     | 0.44              |
| 25:CY:20:A:C8      | 25:CY:47:C:N4     | 2.85                     | 0.44              |
| 25:CY:7:A:C2       | 25:CY:66:A:C2     | 3.06                     | 0.44              |
| 57:D8:40:GLU:O     | 57:D8:42:ARG:N    | 2.50                     | 0.44              |
| 27:DA:1000:A:H3'   | 27:DA:1001:A:C8   | 2.53                     | 0.44              |
| 27:DA:1287:A:C2'   | 27:DA:1288:U:O5'  | 2.65                     | 0.44              |
| 27:DA:1592:C:H2'   | 27:DA:1593:G:O4'  | 2.18                     | 0.44              |
| 27:DA:1663:C:O2'   | 27:DA:1664:A:H5'  | 2.18                     | 0.44              |
| 27:DA:2054:A:C2    | 27:DA:2616:C:C2   | 3.06                     | 0.44              |
| 27:DA:2130:U:C2    | 27:DA:2159:G:O6   | 2.71                     | 0.44              |
| 27:DA:227:A:C2     | 27:DA:2407:G:H1'  | 2.52                     | 0.44              |
| 27:DA:2836:U:O5'   | 27:DA:2836:U:H6   | 2.01                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:286:C:H2'   | 27:DA:287:C:H5'    | 1.98                     | 0.44              |
| 27:DA:2881:C:C2'  | 27:DA:2882:A:H5'   | 2.48                     | 0.44              |
| 27:DA:864:G:H2'   | 27:DA:865:C:H6     | 1.82                     | 0.44              |
| 28:DB:11:C:H3'    | 28:DB:12:C:C6      | 2.53                     | 0.44              |
| 32:DF:20:LEU:HD22 | 32:DF:203:GLN:HE22 | 1.83                     | 0.44              |
| 35:DI:110:ASP:HA  | 35:DI:111:PRO:HD2  | 1.82                     | 0.44              |
| 35:DI:12:LEU:CB   | 35:DI:19:VAL:HG21  | 2.47                     | 0.44              |
| 35:DI:5:LEU:CD1   | 35:DI:17:GLN:HB3   | 2.42                     | 0.44              |
| 36:DN:100:GLU:O   | 36:DN:104:LYS:HB2  | 2.17                     | 0.44              |
| 36:DN:78:TYR:HB3  | 36:DN:79:PRO:HD2   | 1.98                     | 0.44              |
| 39:DQ:137:TYR:O   | 39:DQ:138:ASP:C    | 2.55                     | 0.44              |
| 40:DR:16:HIS:C    | 40:DR:18:LEU:H     | 2.20                     | 0.44              |
| 47:DY:85:VAL:HG12 | 47:DY:86:ARG:H     | 1.82                     | 0.44              |
| 1:AA:1147:C:H2'   | 1:AA:1148:U:O4'    | 2.17                     | 0.44              |
| 1:AA:189(C):C:H6  | 1:AA:189(C):C:O5'  | 2.00                     | 0.44              |
| 1:AA:246:A:C2     | 1:AA:279:A:N1      | 2.85                     | 0.44              |
| 1:AA:43:C:C2'     | 1:AA:44:G:O5'      | 2.65                     | 0.44              |
| 1:AA:928:G:C2     | 1:AA:1390:U:O2     | 2.71                     | 0.44              |
| 1:AA:935:A:C2     | 1:AA:936:C:C2      | 3.05                     | 0.44              |
| 2:AB:126:GLU:C    | 2:AB:128:GLU:H     | 2.17                     | 0.44              |
| 3:AC:114:PRO:O    | 3:AC:118:GLN:HG3   | 2.17                     | 0.44              |
| 3:AC:165:THR:CG2  | 3:AC:166:GLU:N     | 2.81                     | 0.44              |
| 4:AD:194:LEU:N    | 4:AD:194:LEU:HD22  | 2.33                     | 0.44              |
| 6:AF:28:ARG:O     | 6:AF:32:ASN:CG     | 2.56                     | 0.44              |
| 7:AG:98:SER:O     | 7:AG:99:LEU:C      | 2.55                     | 0.44              |
| 11:AK:12:ARG:HG3  | 11:AK:13:GLN:H     | 1.81                     | 0.44              |
| 13:AM:76:ALA:C    | 13:AM:78:ILE:N     | 2.71                     | 0.44              |
| 13:AM:76:ALA:HA   | 13:AM:79:LYS:CB    | 2.47                     | 0.44              |
| 13:AM:82:MET:CG   | 13:AM:82:MET:O     | 2.66                     | 0.44              |
| 15:AO:74:ASP:C    | 15:AO:76:GLU:H     | 2.20                     | 0.44              |
| 21:AU:13:ILE:HG12 | 21:AU:22:ARG:HE    | 1.83                     | 0.44              |
| 23:AW:34:U:H2'    | 23:AW:35:G:O5'     | 2.17                     | 0.44              |
| 25:AY:23:G:H2'    | 25:AY:24:C:H6      | 1.83                     | 0.44              |
| 50:B1:67:ILE:N    | 50:B1:68:PRO:CD    | 2.75                     | 0.44              |
| 54:B5:31:VAL:HG11 | 54:B5:42:PRO:HB3   | 2.00                     | 0.44              |
| 27:BA:2017:U:H4'  | 54:B5:9:LYS:HE2    | 1.98                     | 0.44              |
| 55:B6:32:ASN:O    | 55:B6:33:LYS:HB2   | 2.17                     | 0.44              |
| 55:B6:48:VAL:HG22 | 55:B6:48:VAL:H     | 1.40                     | 0.44              |
| 27:BA:1024:G:HO2' | 27:BA:1144:G:HO2'  | 1.62                     | 0.44              |
| 27:BA:1265:A:H4'  | 27:BA:1266:G:OP1   | 2.18                     | 0.44              |
| 27:BA:1311:G:C5   | 56:B7:47:ARG:NH2   | 2.86                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1442:G:H2'  | 27:BA:1443:G:C8    | 2.52                     | 0.44              |
| 27:BA:1443:G:O5'  | 27:BA:1443:G:H8    | 2.00                     | 0.44              |
| 27:BA:1453:U:H4'  | 27:BA:1455:G:OP1   | 2.18                     | 0.44              |
| 27:BA:1773:A:H2'  | 27:BA:1774:C:O4'   | 2.18                     | 0.44              |
| 27:BA:2027:G:C6   | 27:BA:2028:U:C4    | 3.06                     | 0.44              |
| 27:BA:2074:U:O2'  | 27:BA:2075:U:H5'   | 2.17                     | 0.44              |
| 27:BA:2127:G:C2   | 27:BA:2128:C:C2    | 3.06                     | 0.44              |
| 27:BA:2286:A:H4'  | 27:BA:2287:A:OP2   | 2.17                     | 0.44              |
| 27:BA:2486:G:H8   | 27:BA:2486:G:O5'   | 2.00                     | 0.44              |
| 27:BA:2525:G:C2   | 27:BA:2526:G:C8    | 3.06                     | 0.44              |
| 27:BA:272:G:O6    | 27:BA:421:U:H2'    | 2.18                     | 0.44              |
| 27:BA:41:C:O2     | 27:BA:41:C:H2'     | 2.17                     | 0.44              |
| 27:BA:911:A:C6    | 39:BQ:9:TYR:CG     | 3.06                     | 0.44              |
| 27:BA:840:C:N3    | 27:BA:939:G:C6     | 2.85                     | 0.44              |
| 28:BB:16:G:H2'    | 28:BB:17:C:H6      | 1.83                     | 0.44              |
| 29:BC:195:ALA:C   | 29:BC:197:GLU:H    | 2.21                     | 0.44              |
| 30:BD:201:HIS:C   | 30:BD:201:HIS:HD1  | 2.21                     | 0.44              |
| 30:BD:205:VAL:O   | 30:BD:207:GLY:N    | 2.50                     | 0.44              |
| 30:BD:2:ALA:O     | 30:BD:3:VAL:O      | 2.35                     | 0.44              |
| 27:BA:1565:C:P    | 30:BD:4:LYS:HZ1    | 2.41                     | 0.44              |
| 32:BF:32:LEU:CD2  | 32:BF:105:VAL:HG13 | 2.40                     | 0.44              |
| 33:BG:138:GLN:HB2 | 33:BG:155:MET:CE   | 2.48                     | 0.44              |
| 36:BN:134:ARG:O   | 36:BN:136:GLU:N    | 2.51                     | 0.44              |
| 36:BN:43:THR:HB   | 36:BN:46:VAL:CG1   | 2.48                     | 0.44              |
| 27:BA:2415:G:C3'  | 38:BP:66:GLY:HA3   | 2.47                     | 0.44              |
| 41:BS:12:PHE:HD1  | 41:BS:14:VAL:HG23  | 1.81                     | 0.44              |
| 41:BS:89:ARG:HB3  | 41:BS:92:TYR:CB    | 2.47                     | 0.44              |
| 42:BT:81:PRO:HD2  | 42:BT:82:LEU:HD11  | 1.98                     | 0.44              |
| 43:BU:71:GLN:HB2  | 43:BU:72:HIS:CD2   | 2.52                     | 0.44              |
| 43:BU:66:ASN:CA   | 43:BU:76:TYR:HB2   | 2.48                     | 0.44              |
| 27:BA:1284:A:H2   | 45:BW:45:TYR:OH    | 2.00                     | 0.44              |
| 47:BY:45:VAL:HG12 | 47:BY:46:LYS:N     | 2.32                     | 0.44              |
| 1:CA:1049:U:C5    | 1:CA:1201:A:O4'    | 2.70                     | 0.44              |
| 1:CA:1099:G:H5'   | 1:CA:1100:C:OP2    | 2.18                     | 0.44              |
| 1:CA:1399:C:N3    | 1:CA:1401:G:C2     | 2.85                     | 0.44              |
| 1:CA:1436:U:H2'   | 1:CA:1437:C:O4'    | 2.18                     | 0.44              |
| 1:CA:793:U:O4     | 1:CA:1517:G:H5''   | 2.18                     | 0.44              |
| 1:CA:133:U:C1'    | 1:CA:230:G:N2      | 2.79                     | 0.44              |
| 1:CA:243:A:C2     | 1:CA:245:C:C2      | 3.06                     | 0.44              |
| 1:CA:894:G:C6     | 1:CA:895:G:C5      | 3.05                     | 0.44              |
| 2:CB:236:TYR:HD2  | 2:CB:239:VAL:CB    | 2.28                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CC:139:GLN:O    | 3:CC:143:GLU:HB2   | 2.18                     | 0.44              |
| 3:CC:147:LYS:HB3  | 3:CC:203:PHE:CD2   | 2.52                     | 0.44              |
| 4:CD:3:ARG:O      | 4:CD:4:TYR:CB      | 2.65                     | 0.44              |
| 6:CF:93:SER:O     | 6:CF:94:GLN:HG3    | 2.18                     | 0.44              |
| 9:CI:48:GLU:HG3   | 9:CI:101:PHE:CZ    | 2.52                     | 0.44              |
| 10:CJ:78:ASN:HD21 | 10:CJ:80:LYS:HB3   | 1.82                     | 0.44              |
| 11:CK:41:THR:HG23 | 11:CK:42:TRP:N     | 2.32                     | 0.44              |
| 1:CA:363:A:H8     | 12:CL:30:ARG:HH21  | 1.64                     | 0.44              |
| 13:CM:6:GLY:O     | 13:CM:7:VAL:HG23   | 2.17                     | 0.44              |
| 16:CP:12:LYS:O    | 16:CP:13:HIS:HB2   | 2.17                     | 0.44              |
| 19:CS:61:TYR:CG   | 19:CS:62:ILE:N     | 2.86                     | 0.44              |
| 57:D8:32:LEU:HB3  | 57:D8:36:LYS:NZ    | 2.33                     | 0.44              |
| 57:D8:54:GLU:HA   | 57:D8:57:ARG:NE    | 2.32                     | 0.44              |
| 27:DA:1300:U:O2'  | 27:DA:1301:A:P     | 2.75                     | 0.44              |
| 27:DA:1491:G:N1   | 27:DA:1492:G:C5    | 2.86                     | 0.44              |
| 27:DA:1614:A:H62  | 45:DW:93:ALA:CB    | 2.16                     | 0.44              |
| 27:DA:1847:A:H5'  | 27:DA:1848:A:OP2   | 2.18                     | 0.44              |
| 27:DA:1896:G:O2'  | 27:DA:1897:G:H5'   | 2.18                     | 0.44              |
| 27:DA:1985:G:N2   | 27:DA:1986:A:H1'   | 2.32                     | 0.44              |
| 27:DA:2066:C:O2'  | 27:DA:2067:G:H5'   | 2.17                     | 0.44              |
| 27:DA:2141:G:H2'  | 27:DA:2142:C:C6    | 2.52                     | 0.44              |
| 27:DA:2146:C:O4'  | 27:DA:2147:G:C5    | 2.71                     | 0.44              |
| 27:DA:214:G:H2'   | 27:DA:215:G:OP2    | 2.18                     | 0.44              |
| 27:DA:2253:G:H2'  | 27:DA:2254:C:C6    | 2.52                     | 0.44              |
| 27:DA:2344:U:C4'  | 27:DA:2345:G:OP1   | 2.65                     | 0.44              |
| 27:DA:246:C:N3    | 27:DA:247:G:C8     | 2.86                     | 0.44              |
| 27:DA:2581:G:N3   | 27:DA:2581:G:H2'   | 2.33                     | 0.44              |
| 27:DA:2801:A:H1'  | 27:DA:2801(A):A:N7 | 2.33                     | 0.44              |
| 27:DA:2848:G:H21  | 27:DA:2867:G:H1'   | 1.83                     | 0.44              |
| 27:DA:321:G:O2'   | 27:DA:340:A:O2'    | 2.28                     | 0.44              |
| 27:DA:422:A:C6    | 27:DA:423:A:C6     | 3.06                     | 0.44              |
| 27:DA:459:U:H5''  | 56:D7:40:TRP:CD2   | 2.52                     | 0.44              |
| 27:DA:463:G:N2    | 27:DA:467:G:C5     | 2.86                     | 0.44              |
| 27:DA:470:A:O2'   | 27:DA:471:A:H5'    | 2.17                     | 0.44              |
| 27:DA:531:C:OP1   | 27:DA:561:G:C2     | 2.70                     | 0.44              |
| 27:DA:627:A:N6    | 38:DP:116:GLY:HA2  | 2.33                     | 0.44              |
| 27:DA:750:A:C2    | 27:DA:753:C:C6     | 3.05                     | 0.44              |
| 28:DB:43:C:H1'    | 33:DG:93:THR:HB    | 1.99                     | 0.44              |
| 28:DB:40:U:H1'    | 28:DB:45:A:H61     | 1.82                     | 0.44              |
| 28:DB:71:C:H2'    | 28:DB:72:G:C5'     | 2.47                     | 0.44              |
| 28:DB:85:G:H2'    | 28:DB:86:G:C8      | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DH:158:HIS:NE2 | 34:DH:170:ARG:O   | 2.50                     | 0.44              |
| 35:DI:10:GLU:HG2  | 35:DI:11:ASN:H    | 1.82                     | 0.44              |
| 35:DI:6:LEU:O     | 35:DI:7:GLU:C     | 2.55                     | 0.44              |
| 38:DP:10:PRO:O    | 38:DP:11:GLY:C    | 2.56                     | 0.44              |
| 38:DP:16:ARG:CZ   | 38:DP:18:ARG:CG   | 2.94                     | 0.44              |
| 40:DR:48:VAL:HA   | 40:DR:51:LEU:CD1  | 2.47                     | 0.44              |
| 42:DT:16:ARG:HB3  | 42:DT:19:LEU:CD1  | 2.42                     | 0.44              |
| 43:DU:38:THR:O    | 43:DU:41:ALA:HB3  | 2.17                     | 0.44              |
| 44:DV:82:ARG:HD2  | 44:DV:82:ARG:N    | 2.33                     | 0.44              |
| 45:DW:20:VAL:HG11 | 45:DW:47:VAL:HG21 | 1.98                     | 0.44              |
| 47:DY:13:VAL:O    | 47:DY:24:VAL:HG13 | 2.18                     | 0.44              |
| 47:DY:54:LYS:CE   | 47:DY:55:TYR:HE2  | 2.31                     | 0.44              |
| 47:DY:45:VAL:CA   | 47:DY:62:GLU:HG2  | 2.47                     | 0.44              |
| 1:AA:1014:A:H3'   | 1:AA:1015:A:C8    | 2.53                     | 0.44              |
| 1:AA:1133:G:H22   | 1:AA:1143:G:H1'   | 1.81                     | 0.44              |
| 1:AA:1261:A:C8    | 1:AA:1275:A:C6    | 3.06                     | 0.44              |
| 1:AA:713:G:N2     | 1:AA:714:G:C2     | 2.86                     | 0.44              |
| 1:AA:979:C:C3'    | 1:AA:980:C:C5'    | 2.88                     | 0.44              |
| 1:AA:992:U:O2     | 1:AA:992:U:H2'    | 2.18                     | 0.44              |
| 2:AB:53:ARG:CZ    | 2:AB:199:TYR:CE2  | 3.00                     | 0.44              |
| 4:AD:101:LEU:HD12 | 4:AD:105:VAL:HG23 | 2.00                     | 0.44              |
| 4:AD:96:LEU:HG    | 4:AD:139:ARG:NH1  | 2.33                     | 0.44              |
| 4:AD:52:SER:O     | 4:AD:53:ASP:C     | 2.55                     | 0.44              |
| 5:AE:101:ILE:CG1  | 5:AE:119:LEU:HD23 | 2.48                     | 0.44              |
| 6:AF:23:LYS:HB3   | 6:AF:23:LYS:HE2   | 1.76                     | 0.44              |
| 6:AF:19:LEU:O     | 6:AF:23:LYS:HG3   | 2.18                     | 0.44              |
| 6:AF:45:LEU:HD11  | 6:AF:57:GLN:OE1   | 2.17                     | 0.44              |
| 7:AG:38:LEU:C     | 7:AG:40:ALA:N     | 2.72                     | 0.44              |
| 8:AH:39:LEU:CB    | 8:AH:45:ILE:HD11  | 2.45                     | 0.44              |
| 10:AJ:75:ILE:HG13 | 10:AJ:76:ASN:N    | 2.32                     | 0.44              |
| 10:AJ:81:THR:C    | 10:AJ:83:GLU:H    | 2.21                     | 0.44              |
| 12:AL:21:VAL:HG13 | 12:AL:95:TYR:HE2  | 1.82                     | 0.44              |
| 13:AM:91:ARG:HB2  | 13:AM:98:VAL:CG1  | 2.48                     | 0.44              |
| 13:AM:94:ARG:NH2  | 27:BA:887:A:O5'   | 2.50                     | 0.44              |
| 16:AP:43:LYS:HA   | 16:AP:48:TRP:CD1  | 2.52                     | 0.44              |
| 18:AR:40:LEU:O    | 18:AR:41:LYS:C    | 2.56                     | 0.44              |
| 50:B1:86:SER:CB   | 50:B1:89:GLU:HB2  | 2.43                     | 0.44              |
| 51:B2:15:LYS:O    | 51:B2:15:LYS:HG3  | 2.17                     | 0.44              |
| 27:BA:2286:A:N6   | 55:B6:24:GLU:OE2  | 2.51                     | 0.44              |
| 27:BA:1200:C:C2   | 27:BA:1201:C:C5   | 3.05                     | 0.44              |
| 27:BA:1266:G:O4'  | 45:BW:15:ARG:NH2  | 2.51                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1337:G:C4    | 27:BA:1338:G:C8    | 3.06                     | 0.44              |
| 27:BA:1473:G:O2'   | 27:BA:1474:C:H5'   | 2.18                     | 0.44              |
| 27:BA:1975:G:C2'   | 27:BA:1976:U:H5'   | 2.48                     | 0.44              |
| 27:BA:2279:G:N2    | 27:BA:2280:G:H1'   | 2.32                     | 0.44              |
| 27:BA:2388:A:H2'   | 27:BA:2389:G:H5'   | 2.00                     | 0.44              |
| 27:BA:1663:C:O2'   | 27:BA:2686:G:H4'   | 2.17                     | 0.44              |
| 27:BA:2753:A:O2'   | 27:BA:2754:U:H5'   | 2.17                     | 0.44              |
| 27:BA:318:C:O2'    | 27:BA:319:C:H5'    | 2.17                     | 0.44              |
| 27:BA:324:A:H2'    | 27:BA:325:G:O4'    | 2.17                     | 0.44              |
| 27:BA:702:G:N2     | 27:BA:703:U:C2     | 2.86                     | 0.44              |
| 27:BA:772:C:H2'    | 27:BA:773:U:H6     | 1.83                     | 0.44              |
| 27:BA:852:G:O2'    | 52:B3:41:PRO:HB3   | 2.18                     | 0.44              |
| 27:BA:941:A:C6     | 27:BA:942:G:C6     | 3.05                     | 0.44              |
| 30:BD:138:VAL:HG22 | 30:BD:139:GLY:N    | 2.32                     | 0.44              |
| 30:BD:28:GLU:OE1   | 30:BD:29:PRO:HD2   | 2.17                     | 0.44              |
| 30:BD:76:PRO:HG2   | 30:BD:98:VAL:CG2   | 2.46                     | 0.44              |
| 32:BF:122:LYS:O    | 32:BF:191:ARG:NH1  | 2.50                     | 0.44              |
| 34:BH:54:ARG:HG3   | 34:BH:54:ARG:O     | 2.18                     | 0.44              |
| 34:BH:94:TYR:CD2   | 34:BH:107:VAL:HG12 | 2.52                     | 0.44              |
| 35:BI:91:SER:O     | 35:BI:92:VAL:HG12  | 2.18                     | 0.44              |
| 36:BN:2:LYS:NZ     | 43:BU:95:LEU:CG    | 2.76                     | 0.44              |
| 36:BN:56:ASN:HD22  | 36:BN:56:ASN:HA    | 1.62                     | 0.44              |
| 36:BN:87:LEU:HD21  | 36:BN:98:VAL:CG1   | 2.42                     | 0.44              |
| 40:BR:22:ARG:O     | 40:BR:23:ASN:C     | 2.55                     | 0.44              |
| 40:BR:27:SER:HA    | 40:BR:30:THR:HB    | 2.00                     | 0.44              |
| 43:BU:25:TRP:C     | 43:BU:28:ARG:HB2   | 2.38                     | 0.44              |
| 39:BQ:63:LYS:HD2   | 48:BZ:174:VAL:HG21 | 1.99                     | 0.44              |
| 1:CA:1053:G:C6     | 1:CA:1199:U:C2     | 3.06                     | 0.44              |
| 1:CA:1170:A:H2'    | 1:CA:1171:G:C5'    | 2.48                     | 0.44              |
| 1:CA:1231:G:O2'    | 1:CA:1232:U:H5'    | 2.18                     | 0.44              |
| 1:CA:1252:A:H2'    | 1:CA:1253:G:O4'    | 2.17                     | 0.44              |
| 1:CA:1284:C:H3'    | 1:CA:1285:A:H8     | 1.83                     | 0.44              |
| 1:CA:407:G:H1      | 1:CA:435:C:H42     | 1.64                     | 0.44              |
| 1:CA:723:U:OP1     | 1:CA:723:U:C6      | 2.71                     | 0.44              |
| 1:CA:658:G:C2      | 1:CA:749:C:N3      | 2.86                     | 0.44              |
| 2:CB:142:LEU:HD11  | 2:CB:146:GLN:HE21  | 1.82                     | 0.44              |
| 3:CC:86:VAL:O      | 3:CC:90:GLU:HG2    | 2.18                     | 0.44              |
| 4:CD:142:PRO:HA    | 4:CD:185:PHE:O     | 2.17                     | 0.44              |
| 5:CE:43:LEU:HD21   | 5:CE:132:ALA:HB1   | 2.00                     | 0.44              |
| 6:CF:9:VAL:C       | 6:CF:10:LEU:HD12   | 2.38                     | 0.44              |
| 6:CF:29:ALA:O      | 6:CF:32:ASN:HB2    | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CH:83:ILE:O     | 8:CH:83:ILE:HG23  | 2.18                     | 0.44              |
| 10:CJ:9:ARG:O     | 10:CJ:16:LEU:HG   | 2.18                     | 0.44              |
| 12:CL:82:ILE:HG21 | 12:CL:95:TYR:CD2  | 2.52                     | 0.44              |
| 13:CM:8:GLU:CD    | 13:CM:22:ILE:HG12 | 2.38                     | 0.44              |
| 21:CU:18:TYR:CE2  | 21:CU:22:ARG:NH1  | 2.86                     | 0.44              |
| 52:D3:46:ASN:O    | 52:D3:49:LYS:N    | 2.51                     | 0.44              |
| 27:DA:1278:A:O2'  | 27:DA:1279:G:H5'  | 2.17                     | 0.44              |
| 27:DA:139:G:H2'   | 27:DA:140:G:N7    | 2.33                     | 0.44              |
| 27:DA:1660:C:O2'  | 27:DA:1661:G:H5'  | 2.17                     | 0.44              |
| 27:DA:1721:G:N1   | 27:DA:1739:U:OP2  | 2.51                     | 0.44              |
| 27:DA:1826:G:C4   | 27:DA:1827:C:C5   | 3.05                     | 0.44              |
| 27:DA:1932:A:H2'  | 27:DA:1933:G:H5'  | 2.00                     | 0.44              |
| 27:DA:2397:G:N2   | 27:DA:2398:U:H1'  | 2.31                     | 0.44              |
| 27:DA:2466:C:N4   | 27:DA:2485:G:C6   | 2.86                     | 0.44              |
| 27:DA:2511:U:O4   | 27:DA:2575:C:N3   | 2.51                     | 0.44              |
| 27:DA:10:G:C6     | 27:DA:2629:A:C8   | 3.06                     | 0.44              |
| 27:DA:2808:U:H3'  | 27:DA:2891:G:H1   | 1.83                     | 0.44              |
| 27:DA:2853:C:O2'  | 27:DA:2854:G:H5'  | 2.18                     | 0.44              |
| 27:DA:634:C:O2'   | 27:DA:635:C:O5'   | 2.36                     | 0.44              |
| 27:DA:644:A:H4'   | 27:DA:645:C:H5    | 1.76                     | 0.44              |
| 27:DA:651:G:OP1   | 57:D8:19:SER:OG   | 2.34                     | 0.44              |
| 27:DA:811:U:C2    | 27:DA:1251:C:C5   | 3.06                     | 0.44              |
| 27:DA:84:A:N1     | 27:DA:98:G:C2'    | 2.80                     | 0.44              |
| 27:DA:888:C:C3'   | 27:DA:889:C:H5'   | 2.47                     | 0.44              |
| 27:DA:997:G:C2    | 27:DA:998:C:C4    | 3.06                     | 0.44              |
| 30:DD:122:ASP:C   | 30:DD:122:ASP:OD1 | 2.56                     | 0.44              |
| 30:DD:137:PRO:HB2 | 30:DD:140:THR:CG2 | 2.48                     | 0.44              |
| 35:DI:11:ASN:O    | 35:DI:12:LEU:CB   | 2.62                     | 0.44              |
| 36:DN:55:VAL:HG13 | 36:DN:126:PRO:HB3 | 1.99                     | 0.44              |
| 36:DN:28:THR:CG2  | 36:DN:29:LYS:H    | 2.21                     | 0.44              |
| 37:DO:110:GLY:C   | 37:DO:112:MET:H   | 2.21                     | 0.44              |
| 38:DP:48:PRO:O    | 38:DP:49:ARG:C    | 2.54                     | 0.44              |
| 40:DR:65:LEU:O    | 40:DR:67:LEU:N    | 2.51                     | 0.44              |
| 43:DU:81:HIS:O    | 43:DU:85:LYS:CB   | 2.65                     | 0.44              |
| 45:DW:48:ALA:O    | 45:DW:49:LYS:C    | 2.56                     | 0.44              |
| 45:DW:47:VAL:HA   | 45:DW:50:VAL:CG1  | 2.48                     | 0.44              |
| 1:AA:1443:G:C6    | 1:AA:1460:A:C2    | 3.06                     | 0.44              |
| 1:AA:224:C:H2'    | 1:AA:225:C:C6     | 2.52                     | 0.44              |
| 1:AA:402:G:H4'    | 1:AA:620:C:O2     | 2.18                     | 0.44              |
| 1:AA:442:C:O2     | 1:AA:442:C:H2'    | 2.17                     | 0.44              |
| 1:AA:912:C:O3'    | 12:AL:43:LYS:NZ   | 2.51                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:920:U:O2     | 1:AA:920:U:H2'     | 2.16                     | 0.44              |
| 2:AB:155:LEU:HA   | 2:AB:155:LEU:HD22  | 1.63                     | 0.44              |
| 2:AB:168:THR:HG23 | 2:AB:192:SER:HA    | 2.00                     | 0.44              |
| 2:AB:32:ILE:CG1   | 2:AB:33:TYR:H      | 2.29                     | 0.44              |
| 3:AC:173:VAL:HG12 | 3:AC:175:LEU:CD1   | 2.48                     | 0.44              |
| 4:AD:3:ARG:HG2    | 4:AD:3:ARG:HH21    | 1.82                     | 0.44              |
| 7:AG:88:PRO:HG3   | 7:AG:149:ARG:HA    | 1.99                     | 0.44              |
| 7:AG:62:PHE:O     | 7:AG:65:ALA:HB3    | 2.18                     | 0.44              |
| 9:AI:4:TYR:CA     | 9:AI:88:TYR:CE1    | 2.95                     | 0.44              |
| 10:AJ:3:LYS:N     | 10:AJ:77:PRO:HG3   | 2.33                     | 0.44              |
| 15:AO:66:LEU:C    | 15:AO:68:ARG:N     | 2.70                     | 0.44              |
| 1:AA:230:G:C5'    | 16:AP:23:ASP:OD2   | 2.66                     | 0.44              |
| 20:AT:89:ARG:CD   | 20:AT:104:LEU:HD11 | 2.44                     | 0.44              |
| 23:AW:67:C:O2'    | 23:AW:68:C:H5'     | 2.18                     | 0.44              |
| 51:B2:12:GLU:O    | 51:B2:16:LEU:HD21  | 2.17                     | 0.44              |
| 51:B2:23:LYS:O    | 51:B2:26:ARG:HB2   | 2.18                     | 0.44              |
| 51:B2:38:GLN:HB3  | 51:B2:44:LEU:O     | 2.18                     | 0.44              |
| 55:B6:13:CYS:HB2  | 55:B6:22:ALA:CB    | 2.47                     | 0.44              |
| 27:BA:1048:A:OP2  | 27:BA:1110:G:N2    | 2.38                     | 0.44              |
| 27:BA:1486:A:H2'  | 27:BA:1487:G:C8    | 2.52                     | 0.44              |
| 27:BA:157:U:H2'   | 27:BA:158:U:OP2    | 2.17                     | 0.44              |
| 27:BA:1780:A:H3'  | 27:BA:1781:C:H2'   | 2.00                     | 0.44              |
| 27:BA:1999:C:H1'  | 27:BA:2687:U:O2'   | 2.18                     | 0.44              |
| 27:BA:2388:A:C2'  | 27:BA:2389:G:H5'   | 2.48                     | 0.44              |
| 27:BA:2505:G:C2'  | 27:BA:2506:U:H5'   | 2.47                     | 0.44              |
| 27:BA:2875:C:N3   | 27:BA:2876:G:N7    | 2.65                     | 0.44              |
| 27:BA:310:A:H1'   | 27:BA:311:A:H2'    | 2.00                     | 0.44              |
| 27:BA:353:G:N3    | 27:BA:354:G:C8     | 2.86                     | 0.44              |
| 27:BA:441:U:O2    | 32:BF:46:ARG:NH2   | 2.50                     | 0.44              |
| 27:BA:644:A:O2'   | 27:BA:645:C:H5''   | 2.18                     | 0.44              |
| 27:BA:72:U:H3     | 51:B2:62:THR:HG1   | 1.66                     | 0.44              |
| 27:BA:740:U:H6    | 27:BA:740:U:C5'    | 2.12                     | 0.44              |
| 27:BA:781:A:H2    | 27:BA:1776:G:N3    | 2.16                     | 0.44              |
| 27:BA:861:A:C2    | 27:BA:917:A:C4     | 3.06                     | 0.44              |
| 28:BB:105:A:H2'   | 28:BB:106:G:C4'    | 2.48                     | 0.44              |
| 30:BD:32:SER:HA   | 30:BD:36:PRO:HG3   | 2.00                     | 0.44              |
| 31:BE:100:GLU:O   | 31:BE:172:VAL:CG2  | 2.64                     | 0.44              |
| 27:BA:1658:C:OP1  | 31:BE:132:HIS:CE1  | 2.71                     | 0.44              |
| 31:BE:59:VAL:O    | 31:BE:60:ASN:HB3   | 2.17                     | 0.44              |
| 27:BA:1248:G:OP1  | 32:BF:92:PRO:HB3   | 2.18                     | 0.44              |
| 33:BG:35:GLU:CB   | 33:BG:160:VAL:O    | 2.63                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:BG:32:PRO:O     | 33:BG:33:ARG:HG3  | 2.17                     | 0.44              |
| 34:BH:103:LEU:HD22 | 34:BH:123:PHE:CE2 | 2.52                     | 0.44              |
| 37:BO:3:GLN:HE21   | 37:BO:32:TYR:HD1  | 1.66                     | 0.44              |
| 38:BP:16:ARG:CG    | 38:BP:17:LYS:N    | 2.80                     | 0.44              |
| 38:BP:81:GLN:CG    | 38:BP:82:GLY:N    | 2.80                     | 0.44              |
| 38:BP:99:LEU:O     | 38:BP:99:LEU:HD23 | 2.18                     | 0.44              |
| 41:BS:77:ALA:O     | 41:BS:78:LEU:C    | 2.55                     | 0.44              |
| 42:BT:42:ILE:CD1   | 42:BT:42:ILE:O    | 2.65                     | 0.44              |
| 43:BU:72:HIS:N     | 43:BU:72:HIS:CD2  | 2.85                     | 0.44              |
| 43:BU:83:LEU:CD1   | 43:BU:113:ALA:HB2 | 2.47                     | 0.44              |
| 44:BV:46:VAL:CG2   | 44:BV:47:VAL:H    | 2.12                     | 0.44              |
| 1:CA:1255:G:N2     | 1:CA:1259:C:O2    | 2.50                     | 0.44              |
| 1:CA:1493:A:OP2    | 26:CZ:6:5OH:NP    | 2.50                     | 0.44              |
| 1:CA:380:G:N2      | 1:CA:384:G:C5     | 2.86                     | 0.44              |
| 1:CA:390:C:O3'     | 16:CP:28:ARG:NH2  | 2.50                     | 0.44              |
| 1:CA:529:G:H4'     | 1:CA:533:A:C2     | 2.53                     | 0.44              |
| 1:CA:582:U:C2      | 1:CA:760:G:C6     | 3.06                     | 0.44              |
| 1:CA:748:C:O2'     | 1:CA:749:C:P      | 2.76                     | 0.44              |
| 1:CA:978:A:H3'     | 1:CA:979:C:C5     | 2.52                     | 0.44              |
| 2:CB:9:GLU:HA      | 2:CB:12:GLU:OE1   | 2.17                     | 0.44              |
| 3:CC:182:ILE:HD11  | 3:CC:203:PHE:CD1  | 2.51                     | 0.44              |
| 5:CE:127:ASN:O     | 5:CE:131:ILE:HG12 | 2.17                     | 0.44              |
| 5:CE:140:ARG:O     | 5:CE:143:ARG:NH2  | 2.51                     | 0.44              |
| 6:CF:93:SER:O      | 6:CF:94:GLN:CG    | 2.66                     | 0.44              |
| 7:CG:151:TYR:OH    | 11:CK:54:ARG:HD3  | 2.18                     | 0.44              |
| 7:CG:43:PHE:O      | 7:CG:46:ALA:HB3   | 2.18                     | 0.44              |
| 8:CH:129:VAL:HB    | 8:CH:130:GLY:H    | 1.72                     | 0.44              |
| 8:CH:133:LEU:HD23  | 8:CH:133:LEU:C    | 2.37                     | 0.44              |
| 8:CH:90:GLY:O      | 8:CH:91:ARG:HB2   | 2.17                     | 0.44              |
| 17:CQ:64:PRO:HA    | 17:CQ:70:ARG:CG   | 2.47                     | 0.44              |
| 1:CA:133:U:OP1     | 20:CT:74:LYS:HE2  | 2.17                     | 0.44              |
| 24:CX:10:G:H2'     | 24:CX:11:A:C8     | 2.52                     | 0.44              |
| 50:D1:5:CYS:SG     | 50:D1:62:VAL:HG23 | 2.58                     | 0.44              |
| 51:D2:21:LEU:O     | 51:D2:22:GLU:C    | 2.56                     | 0.44              |
| 57:D8:13:ARG:O     | 57:D8:14:VAL:HB   | 2.18                     | 0.44              |
| 27:DA:2528:U:C5'   | 58:D9:31:LYS:HE2  | 2.48                     | 0.44              |
| 27:DA:941:A:O2'    | 27:DA:1190:G:H4'  | 2.18                     | 0.44              |
| 27:DA:1303:G:N2    | 27:DA:1304:C:C2   | 2.86                     | 0.44              |
| 27:DA:1332:G:C4'   | 27:DA:1333:C:OP2  | 2.66                     | 0.44              |
| 27:DA:1460:A:O2'   | 27:DA:1461:G:OP1  | 2.32                     | 0.44              |
| 27:DA:150:C:H2'    | 27:DA:151:C:H6    | 1.81                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:1624:G:H2'   | 27:DA:1625:C:C6   | 2.52                     | 0.44              |
| 27:DA:1625:C:O2'   | 27:DA:1626:G:H5'  | 2.18                     | 0.44              |
| 27:DA:1658:C:OP1   | 31:DE:132:HIS:CE1 | 2.71                     | 0.44              |
| 27:DA:154:G:C6     | 27:DA:173:G:C6    | 3.06                     | 0.44              |
| 27:DA:1858:G:O2'   | 27:DA:1859:A:H8   | 2.01                     | 0.44              |
| 27:DA:1906:G:C2    | 27:DA:1925:C:O2   | 2.71                     | 0.44              |
| 27:DA:245:G:C4     | 27:DA:246:C:C5    | 3.05                     | 0.44              |
| 27:DA:2605:U:H2'   | 27:DA:2606:C:C5   | 2.51                     | 0.44              |
| 27:DA:2637:U:H1'   | 27:DA:2782:G:N2   | 2.33                     | 0.44              |
| 27:DA:2657:A:H2'   | 27:DA:2658:C:O4'  | 2.17                     | 0.44              |
| 27:DA:2714:G:C5    | 27:DA:2715:C:C5   | 3.06                     | 0.44              |
| 27:DA:2768:C:N4    | 27:DA:2769:C:N4   | 2.66                     | 0.44              |
| 27:DA:312:G:C4     | 27:DA:313:C:C5    | 3.06                     | 0.44              |
| 27:DA:766:C:O2'    | 27:DA:767:U:H5'   | 2.17                     | 0.44              |
| 28:DB:14:U:O3'     | 28:DB:108:U:O2'   | 2.32                     | 0.44              |
| 29:DC:77:ILE:CG2   | 29:DC:123:VAL:N   | 2.81                     | 0.44              |
| 30:DD:146:GLU:CB   | 30:DD:152:GLY:O   | 2.65                     | 0.44              |
| 30:DD:206:LEU:HD22 | 30:DD:211:ARG:CG  | 2.48                     | 0.44              |
| 31:DE:25:VAL:C     | 31:DE:26:ILE:HD13 | 2.38                     | 0.44              |
| 31:DE:77:ILE:C     | 31:DE:78:LEU:HD23 | 2.38                     | 0.44              |
| 32:DF:18:ARG:O     | 32:DF:19:GLU:HB3  | 2.18                     | 0.44              |
| 32:DF:3:GLU:CB     | 32:DF:24:LEU:HG   | 2.48                     | 0.44              |
| 32:DF:68:LYS:HG3   | 32:DF:69:HIS:CE1  | 2.53                     | 0.44              |
| 33:DG:101:ILE:CD1  | 33:DG:105:LYS:NZ  | 2.79                     | 0.44              |
| 33:DG:129:GLY:O    | 33:DG:161:THR:N   | 2.51                     | 0.44              |
| 34:DH:143:GLN:NE2  | 34:DH:147:ASN:ND2 | 2.65                     | 0.44              |
| 34:DH:54:ARG:O     | 34:DH:54:ARG:CG   | 2.65                     | 0.44              |
| 34:DH:64:LEU:C     | 34:DH:66:GLY:H    | 2.20                     | 0.44              |
| 36:DN:125:GLY:HA3  | 36:DN:126:PRO:C   | 2.38                     | 0.44              |
| 37:DO:38:VAL:HG22  | 37:DO:111:PHE:HZ  | 1.83                     | 0.44              |
| 39:DQ:73:PRO:HA    | 39:DQ:93:TYR:CD2  | 2.53                     | 0.44              |
| 42:DT:11:GLU:C     | 42:DT:13:ARG:H    | 2.17                     | 0.44              |
| 43:DU:24:TYR:HD1   | 43:DU:28:ARG:O    | 2.01                     | 0.44              |
| 43:DU:87:GLY:O     | 44:DV:50:PRO:CD   | 2.56                     | 0.44              |
| 43:DU:83:LEU:O     | 43:DU:88:ILE:N    | 2.51                     | 0.44              |
| 44:DV:68:LYS:NZ    | 44:DV:68:LYS:HA   | 2.32                     | 0.44              |
| 1:AA:984:C:N3      | 1:AA:1222:G:C2    | 2.86                     | 0.44              |
| 1:AA:1231:G:H2'    | 1:AA:1232:U:O4'   | 2.18                     | 0.44              |
| 1:AA:1305:G:O2'    | 1:AA:1306:A:C8    | 2.70                     | 0.44              |
| 1:AA:1520:G:H2'    | 1:AA:1521:G:H8    | 1.82                     | 0.44              |
| 1:AA:203:U:C6      | 1:AA:203:U:OP2    | 2.69                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:609:A:O2'    | 1:AA:610:G:H5'    | 2.16                     | 0.44              |
| 1:AA:758:G:H4'    | 1:AA:880:C:H4'    | 2.00                     | 0.44              |
| 2:AB:16:HIS:HD2   | 2:AB:210:SER:HA   | 1.81                     | 0.44              |
| 2:AB:236:TYR:O    | 2:AB:237:ALA:C    | 2.56                     | 0.44              |
| 3:AC:120:VAL:HA   | 3:AC:123:GLN:HG3  | 2.00                     | 0.44              |
| 4:AD:138:TYR:CE2  | 4:AD:139:ARG:O    | 2.71                     | 0.44              |
| 5:AE:109:ILE:HD13 | 5:AE:136:MET:SD   | 2.57                     | 0.44              |
| 5:AE:12:LEU:HD22  | 5:AE:13:ILE:N     | 2.33                     | 0.44              |
| 6:AF:50:TYR:CZ    | 18:AR:77:GLY:HA2  | 2.53                     | 0.44              |
| 1:AA:640:A:N3     | 8:AH:115:SER:CB   | 2.81                     | 0.44              |
| 9:AI:27:THR:HG23  | 9:AI:31:GLN:O     | 2.17                     | 0.44              |
| 1:AA:1291:G:O2'   | 9:AI:38:GLN:HB3   | 2.18                     | 0.44              |
| 12:AL:22:PRO:C    | 12:AL:24:LEU:H    | 2.16                     | 0.44              |
| 17:AQ:56:VAL:O    | 17:AQ:77:VAL:HG23 | 2.18                     | 0.44              |
| 20:AT:53:LEU:HD22 | 20:AT:56:MET:CE   | 2.48                     | 0.44              |
| 25:AY:29:G:H2'    | 25:AY:30:A:H8     | 1.83                     | 0.44              |
| 40:BR:99:LYS:NZ   | 54:B5:43:HIS:HB3  | 2.32                     | 0.44              |
| 27:BA:643:A:N7    | 55:B6:42:TRP:CH2  | 2.86                     | 0.44              |
| 55:B6:9:LEU:C     | 55:B6:9:LEU:HD23  | 2.37                     | 0.44              |
| 27:BA:1018:C:C2'  | 27:BA:1018:C:O2   | 2.63                     | 0.44              |
| 27:BA:1018:C:O3'  | 27:BA:1120:G:N2   | 2.51                     | 0.44              |
| 27:BA:1278:A:N1   | 27:BA:1279:G:C5   | 2.86                     | 0.44              |
| 27:BA:1399:C:O2'  | 27:BA:1400:G:H5'  | 2.18                     | 0.44              |
| 27:BA:1433:U:H5'' | 27:BA:1433:U:C6   | 2.50                     | 0.44              |
| 27:BA:1465:G:N2   | 27:BA:1466:G:H1'  | 2.32                     | 0.44              |
| 27:BA:1472:A:O2'  | 27:BA:1473:G:H5'  | 2.18                     | 0.44              |
| 27:BA:1448:G:H1'  | 27:BA:1528:A:H62  | 1.82                     | 0.44              |
| 27:BA:1892:C:C2'  | 27:BA:1893:C:H5'  | 2.47                     | 0.44              |
| 27:BA:2476:A:C3'  | 27:BA:2477:C:H5'' | 2.48                     | 0.44              |
| 27:BA:2539:C:C4   | 27:BA:2540:C:C5   | 3.06                     | 0.44              |
| 27:BA:2615:U:N1   | 54:B5:7:PRO:HA    | 2.33                     | 0.44              |
| 27:BA:2639:A:C2'  | 27:BA:2640:G:H5'  | 2.48                     | 0.44              |
| 27:BA:2702:U:H1'  | 27:BA:2703:C:C5   | 2.53                     | 0.44              |
| 27:BA:2727:G:C2   | 27:BA:2728:U:C4   | 3.06                     | 0.44              |
| 27:BA:2804:C:C2'  | 27:BA:2805:G:C8   | 3.01                     | 0.44              |
| 27:BA:887:A:H2'   | 27:BA:887:A:N3    | 2.32                     | 0.44              |
| 27:BA:919:G:C2'   | 27:BA:920:G:H5'   | 2.48                     | 0.44              |
| 27:BA:953:A:C2    | 27:BA:965:C:O2    | 2.71                     | 0.44              |
| 28:BB:14:U:OP2    | 28:BB:70:C:O2'    | 2.23                     | 0.44              |
| 30:BD:3:VAL:HG13  | 30:BD:4:LYS:O     | 2.17                     | 0.44              |
| 31:BE:76:ARG:O    | 31:BE:77:ILE:O    | 2.36                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:BH:20:ALA:O     | 34:BH:21:PRO:O    | 2.35                     | 0.44              |
| 34:BH:72:ILE:O     | 34:BH:76:VAL:HG23 | 2.18                     | 0.44              |
| 35:BI:77:LEU:HD22  | 35:BI:78:THR:N    | 2.33                     | 0.44              |
| 35:BI:94:ALA:O     | 35:BI:97:ILE:N    | 2.51                     | 0.44              |
| 36:BN:75:TYR:HA    | 36:BN:81:GLY:O    | 2.18                     | 0.44              |
| 37:BO:105:GLU:O    | 37:BO:108:GLU:HB2 | 2.18                     | 0.44              |
| 38:BP:49:ARG:O     | 57:B8:55:ALA:HB1  | 2.18                     | 0.44              |
| 31:BE:52:LEU:CD1   | 42:BT:1:MET:HE1   | 2.48                     | 0.44              |
| 42:BT:28:VAL:CG2   | 42:BT:47:GLY:N    | 2.62                     | 0.44              |
| 44:BV:17:GLY:HA2   | 44:BV:96:ILE:O    | 2.18                     | 0.44              |
| 40:BR:103:ARG:HH11 | 45:BW:40:ASN:ND2  | 2.15                     | 0.44              |
| 47:BY:77:PRO:O     | 47:BY:78:ALA:CB   | 2.64                     | 0.44              |
| 47:BY:88:LYS:HZ3   | 47:BY:93:GLY:CA   | 2.17                     | 0.44              |
| 48:BZ:152:SER:HB2  | 48:BZ:166:PRO:HB3 | 1.98                     | 0.44              |
| 1:CA:1033:G:H2'    | 1:CA:1034:G:O4'   | 2.18                     | 0.44              |
| 1:CA:1092:A:H2'    | 1:CA:1093:A:C8    | 2.53                     | 0.44              |
| 1:CA:1273:G:H3'    | 1:CA:1274:G:C8    | 2.53                     | 0.44              |
| 1:CA:319:G:H2'     | 1:CA:319:G:N3     | 2.33                     | 0.44              |
| 1:CA:815:A:H5'     | 1:CA:816:A:O5'    | 2.18                     | 0.44              |
| 1:CA:568:G:N2      | 1:CA:883:C:N1     | 2.66                     | 0.44              |
| 2:CB:132:LYS:HA    | 2:CB:135:GLN:CB   | 2.48                     | 0.44              |
| 5:CE:12:LEU:HD13   | 5:CE:13:ILE:N     | 2.33                     | 0.44              |
| 5:CE:95:ALA:O      | 5:CE:96:PRO:C     | 2.56                     | 0.44              |
| 6:CF:97:PHE:O      | 18:CR:31:LEU:CD2  | 2.66                     | 0.44              |
| 7:CG:146:GLU:HA    | 7:CG:149:ARG:HB2  | 1.99                     | 0.44              |
| 8:CH:86:ILE:O      | 8:CH:87:SER:C     | 2.54                     | 0.44              |
| 13:CM:66:LEU:CD1   | 13:CM:66:LEU:N    | 2.81                     | 0.44              |
| 14:CN:41:ARG:HG2   | 14:CN:41:ARG:HH11 | 1.82                     | 0.44              |
| 14:CN:47:LEU:O     | 14:CN:48:ALA:C    | 2.56                     | 0.44              |
| 17:CQ:6:LEU:N      | 17:CQ:6:LEU:HD12  | 2.33                     | 0.44              |
| 19:CS:11:VAL:HG13  | 19:CS:11:VAL:O    | 2.18                     | 0.44              |
| 1:CA:192:U:C1'     | 20:CT:103:GLY:CA  | 2.95                     | 0.44              |
| 23:CW:31:U:H2'     | 23:CW:32:U:H6     | 1.83                     | 0.44              |
| 1:CA:1492:A:H5'    | 26:CZ:6:5OH:NP    | 2.32                     | 0.44              |
| 51:D2:64:LEU:C     | 51:D2:64:LEU:HD23 | 2.38                     | 0.44              |
| 51:D2:65:ASN:O     | 51:D2:68:ARG:N    | 2.49                     | 0.44              |
| 54:D5:23:HIS:O     | 54:D5:24:ALA:C    | 2.55                     | 0.44              |
| 55:D6:35:GLU:HB3   | 55:D6:51:GLU:HG2  | 1.99                     | 0.44              |
| 27:DA:1010:A:O2'   | 27:DA:1011:G:C5'  | 2.66                     | 0.44              |
| 27:DA:1394:U:C4    | 27:DA:1395:A:C6   | 3.06                     | 0.44              |
| 27:DA:1547:C:O2'   | 27:DA:1548:C:H5'  | 2.17                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:1620:G:C6    | 27:DA:1621:U:C4   | 3.05                     | 0.44              |
| 27:DA:188:G:H2'    | 27:DA:189:G:O4'   | 2.18                     | 0.44              |
| 27:DA:1998:G:O2'   | 27:DA:1999:C:H5'  | 2.18                     | 0.44              |
| 27:DA:2043:C:N3    | 27:DA:2044:C:C5   | 2.86                     | 0.44              |
| 27:DA:2263:C:N4    | 27:DA:2278:A:N6   | 2.66                     | 0.44              |
| 27:DA:2340:G:O2'   | 27:DA:2341:G:H5'  | 2.18                     | 0.44              |
| 27:DA:2365:G:HO2'  | 27:DA:2366:A:H8   | 1.62                     | 0.44              |
| 27:DA:2428:G:H4'   | 27:DA:2429:G:C5   | 2.53                     | 0.44              |
| 27:DA:258:G:O2'    | 27:DA:259:G:H5'   | 2.18                     | 0.44              |
| 27:DA:2832:U:O2'   | 27:DA:2833:G:OP2  | 2.33                     | 0.44              |
| 27:DA:370:G:HO2'   | 27:DA:371:A:P     | 2.41                     | 0.44              |
| 27:DA:481:G:N2     | 27:DA:507:A:C8    | 2.86                     | 0.44              |
| 27:DA:675:A:H4'    | 32:DF:67:GLN:CD   | 2.38                     | 0.44              |
| 27:DA:781:A:H2     | 27:DA:1776:G:N3   | 2.16                     | 0.44              |
| 27:DA:7:G:H5''     | 36:DN:121:LYS:HZ3 | 1.82                     | 0.44              |
| 29:DC:36:LYS:CB    | 29:DC:36:LYS:NZ   | 2.79                     | 0.44              |
| 30:DD:143:HIS:HA   | 30:DD:156:ALA:HB1 | 2.00                     | 0.44              |
| 32:DF:187:VAL:CG1  | 38:DP:7:ARG:NH2   | 2.74                     | 0.44              |
| 33:DG:111:LEU:HD21 | 33:DG:120:LEU:CD2 | 2.48                     | 0.44              |
| 33:DG:167:GLU:HA   | 33:DG:170:ARG:HB3 | 1.99                     | 0.44              |
| 33:DG:41:GLN:HG2   | 33:DG:155:MET:CB  | 2.48                     | 0.44              |
| 33:DG:96:ARG:O     | 33:DG:97:ASP:C    | 2.55                     | 0.44              |
| 34:DH:127:GLU:O    | 34:DH:129:THR:N   | 2.51                     | 0.44              |
| 35:DI:30:LEU:HD23  | 35:DI:35:LEU:HD12 | 1.99                     | 0.44              |
| 38:DP:107:LYS:C    | 38:DP:109:GLY:H   | 2.21                     | 0.44              |
| 32:DF:117:ARG:CZ   | 38:DP:5:ASP:N     | 2.81                     | 0.44              |
| 38:DP:85:LEU:N     | 38:DP:115:LEU:O   | 2.51                     | 0.44              |
| 45:DW:83:LYS:CA    | 45:DW:97:LYS:HG2  | 2.43                     | 0.44              |
| 48:DZ:101:LEU:N    | 48:DZ:121:ARG:O   | 2.51                     | 0.44              |
| 48:DZ:124:LEU:HD12 | 48:DZ:125:VAL:N   | 2.30                     | 0.44              |
| 1:AA:1073:U:OP2    | 5:AE:57:LYS:NZ    | 2.50                     | 0.43              |
| 1:AA:1151:A:O2'    | 1:AA:1152:A:O5'   | 2.36                     | 0.43              |
| 1:AA:1245:A:O2'    | 1:AA:1246:C:H5'   | 2.17                     | 0.43              |
| 1:AA:1349:A:O2'    | 1:AA:1350:A:H5'   | 2.18                     | 0.43              |
| 1:AA:1408:A:C2'    | 1:AA:1409:C:H5'   | 2.47                     | 0.43              |
| 1:AA:408:A:C2      | 1:AA:409:G:C4     | 3.05                     | 0.43              |
| 1:AA:573:A:N3      | 1:AA:883:C:O2'    | 2.43                     | 0.43              |
| 1:AA:573:A:C2      | 1:AA:574:A:C2     | 3.06                     | 0.43              |
| 1:AA:589:C:H6      | 1:AA:589:C:O5'    | 2.00                     | 0.43              |
| 1:AA:606:G:O2'     | 1:AA:631:G:N2     | 2.51                     | 0.43              |
| 1:AA:992:U:HO2'    | 1:AA:993:G:H5''   | 1.82                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:187:LEU:HD23  | 2:AB:201:ILE:O    | 2.18                     | 0.43              |
| 2:AB:204:ASN:HD21  | 2:AB:206:ASP:N    | 2.16                     | 0.43              |
| 2:AB:235:SER:OG    | 2:AB:236:TYR:HD1  | 2.01                     | 0.43              |
| 3:AC:42:LEU:O      | 3:AC:45:LYS:N     | 2.50                     | 0.43              |
| 4:AD:10:ARG:HH11   | 4:AD:10:ARG:CG    | 2.30                     | 0.43              |
| 7:AG:116:ALA:HA    | 7:AG:119:ARG:NE   | 2.25                     | 0.43              |
| 7:AG:116:ALA:HB2   | 7:AG:119:ARG:HH21 | 1.83                     | 0.43              |
| 7:AG:4:ARG:HH11    | 7:AG:5:ARG:HH12   | 1.64                     | 0.43              |
| 8:AH:2:LEU:HD22    | 8:AH:3:THR:N      | 2.32                     | 0.43              |
| 11:AK:120:ARG:HA   | 11:AK:121:PRO:HD3 | 1.84                     | 0.43              |
| 15:AO:12:ILE:C     | 15:AO:14:GLU:H    | 2.20                     | 0.43              |
| 16:AP:26:ARG:HH12  | 16:AP:31:LYS:HD3  | 1.83                     | 0.43              |
| 17:AQ:18:THR:CG2   | 17:AQ:69:LYS:HE3  | 2.26                     | 0.43              |
| 18:AR:59:SER:O     | 18:AR:61:LYS:N    | 2.50                     | 0.43              |
| 22:AV:4:A:H2'      | 22:AV:5:U:O4'     | 2.17                     | 0.43              |
| 23:AW:10:G:H22     | 23:AW:25:A:H1'    | 1.81                     | 0.43              |
| 51:B2:55:ARG:C     | 51:B2:57:ILE:N    | 2.68                     | 0.43              |
| 53:B4:54:LYS:C     | 53:B4:56:GLU:H    | 2.22                     | 0.43              |
| 55:B6:40:CYS:HA    | 55:B6:41:PRO:HD3  | 1.74                     | 0.43              |
| 57:B8:51:ALA:C     | 57:B8:53:PRO:CD   | 2.83                     | 0.43              |
| 27:BA:1310:G:H2'   | 27:BA:1311:G:C5'  | 2.48                     | 0.43              |
| 27:BA:1328:G:O2'   | 27:BA:1329:U:H2'  | 2.18                     | 0.43              |
| 27:BA:1387:C:H2'   | 27:BA:1388:G:H8   | 1.83                     | 0.43              |
| 27:BA:1506:C:O2    | 27:BA:1506:C:H2'  | 2.16                     | 0.43              |
| 27:BA:1549:C:H4'   | 27:BA:1742:G:H21  | 1.82                     | 0.43              |
| 27:BA:2000:G:O2'   | 27:BA:2001:A:H5'  | 2.18                     | 0.43              |
| 27:BA:2105:C:C2'   | 27:BA:2106:G:H5'  | 2.47                     | 0.43              |
| 27:BA:2282:G:H4'   | 27:BA:2283:C:O5'  | 2.18                     | 0.43              |
| 27:BA:2306:C:C6    | 27:BA:2307:G:H1'  | 2.53                     | 0.43              |
| 27:BA:2436:G:H2'   | 27:BA:2437:U:C6   | 2.53                     | 0.43              |
| 27:BA:2511:U:C2'   | 27:BA:2512:C:H5'  | 2.47                     | 0.43              |
| 27:BA:2748:A:H8    | 27:BA:2754:U:O4   | 2.01                     | 0.43              |
| 27:BA:458:G:H1'    | 27:BA:459:U:H5    | 1.82                     | 0.43              |
| 28:BB:105:A:C8     | 28:BB:106:G:C8    | 3.06                     | 0.43              |
| 29:BC:85:GLU:O     | 29:BC:152:ILE:O   | 2.36                     | 0.43              |
| 29:BC:45:ALA:O     | 29:BC:46:LYS:CB   | 2.65                     | 0.43              |
| 33:BG:111:LEU:N    | 33:BG:112:PRO:CD  | 2.80                     | 0.43              |
| 35:BI:31:LEU:N     | 35:BI:31:LEU:CD1  | 2.81                     | 0.43              |
| 35:BI:92:VAL:O     | 35:BI:92:VAL:HG13 | 2.16                     | 0.43              |
| 38:BP:115:LEU:HD23 | 38:BP:115:LEU:N   | 2.33                     | 0.43              |
| 38:BP:16:ARG:CZ    | 38:BP:18:ARG:CG   | 2.84                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BR:87:TYR:HB3  | 40:BR:90:ARG:HB3   | 2.01                     | 0.43              |
| 41:BS:71:ARG:O    | 41:BS:74:ALA:HB3   | 2.18                     | 0.43              |
| 42:BT:52:ILE:HA   | 42:BT:61:PHE:HA    | 2.00                     | 0.43              |
| 42:BT:7:ILE:O     | 42:BT:10:VAL:N     | 2.51                     | 0.43              |
| 44:BV:38:LEU:C    | 44:BV:38:LEU:CD2   | 2.77                     | 0.43              |
| 44:BV:39:LEU:N    | 44:BV:39:LEU:HD13  | 2.33                     | 0.43              |
| 46:BX:12:VAL:CG1  | 46:BX:27:THR:OG1   | 2.62                     | 0.43              |
| 47:BY:46:LYS:HB3  | 47:BY:47:LYS:H     | 1.69                     | 0.43              |
| 1:CA:1002:G:H5''  | 1:CA:1003:G:OP2    | 2.18                     | 0.43              |
| 1:CA:1086:U:O2'   | 1:CA:1087:G:H5'    | 2.18                     | 0.43              |
| 1:CA:1068:G:C8    | 1:CA:1094:G:H8     | 2.35                     | 0.43              |
| 1:CA:1316:G:H2'   | 1:CA:1317:C:H5''   | 2.00                     | 0.43              |
| 1:CA:147:G:H2'    | 1:CA:148:G:C8      | 2.52                     | 0.43              |
| 1:CA:232:G:C4     | 1:CA:233:C:C5      | 3.06                     | 0.43              |
| 1:CA:301:G:H2'    | 1:CA:302:G:C8      | 2.53                     | 0.43              |
| 1:CA:426:G:H2'    | 1:CA:427:U:H6      | 1.80                     | 0.43              |
| 1:CA:472:A:H4'    | 16:CP:80:PHE:O     | 2.18                     | 0.43              |
| 1:CA:631:G:H5''   | 1:CA:632:A:OP1     | 2.16                     | 0.43              |
| 2:CB:31:TYR:O     | 2:CB:32:ILE:HB     | 2.18                     | 0.43              |
| 3:CC:92:ALA:CA    | 3:CC:99:VAL:HG11   | 2.48                     | 0.43              |
| 4:CD:135:LEU:HA   | 4:CD:136:PRO:HD3   | 1.87                     | 0.43              |
| 5:CE:28:PHE:CE1   | 5:CE:49:PRO:O      | 2.71                     | 0.43              |
| 5:CE:9:LYS:HB3    | 5:CE:112:LEU:HD11  | 2.00                     | 0.43              |
| 9:CI:40:LEU:O     | 9:CI:42:ARG:N      | 2.49                     | 0.43              |
| 11:CK:48:ILE:HD11 | 11:CK:67:ASP:HB2   | 2.00                     | 0.43              |
| 18:CR:67:ALA:C    | 18:CR:69:THR:H     | 2.20                     | 0.43              |
| 20:CT:100:ILE:H   | 20:CT:100:ILE:HD12 | 1.79                     | 0.43              |
| 22:CV:1:A:C2'     | 22:CV:2:A:H5'      | 2.47                     | 0.43              |
| 23:CW:8:U:H3'     | 23:CW:13:A:N6      | 2.33                     | 0.43              |
| 51:D2:53:LEU:O    | 51:D2:54:LYS:C     | 2.55                     | 0.43              |
| 51:D2:65:ASN:HB3  | 51:D2:69:ARG:HH12  | 1.83                     | 0.43              |
| 52:D3:7:LYS:CG    | 52:D3:8:LEU:N      | 2.70                     | 0.43              |
| 52:D3:8:LEU:HB3   | 52:D3:31:LEU:HA    | 2.00                     | 0.43              |
| 55:D6:9:LEU:HD23  | 55:D6:10:LEU:N     | 2.33                     | 0.43              |
| 27:DA:1033:U:OP1  | 58:D9:16:VAL:HG21  | 2.18                     | 0.43              |
| 27:DA:1044:G:H1'  | 27:DA:1111:A:N1    | 2.31                     | 0.43              |
| 27:DA:1165:U:H3   | 27:DA:1184:G:H1    | 1.65                     | 0.43              |
| 27:DA:1184:G:C6   | 27:DA:1185:C:N4    | 2.86                     | 0.43              |
| 27:DA:1210:A:P    | 27:DA:1212:G:H5'   | 2.58                     | 0.43              |
| 27:DA:1324:G:C2   | 27:DA:1331:A:N1    | 2.86                     | 0.43              |
| 27:DA:1392:A:C6   | 27:DA:1393:A:N1    | 2.86                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:1401:G:H2'   | 27:DA:1402:C:H6    | 1.81                     | 0.43              |
| 27:DA:1504:C:C3'   | 27:DA:1505:C:H5''  | 2.44                     | 0.43              |
| 27:DA:1485:G:N2    | 27:DA:1505:C:N3    | 2.57                     | 0.43              |
| 27:DA:1562:A:H2'   | 27:DA:1563:G:C8    | 2.53                     | 0.43              |
| 27:DA:2114:A:C2    | 27:DA:2168:G:O4'   | 2.68                     | 0.43              |
| 27:DA:2274:A:C5    | 27:DA:2276:G:C8    | 3.06                     | 0.43              |
| 27:DA:2321:G:C2'   | 27:DA:2321:G:N3    | 2.80                     | 0.43              |
| 27:DA:2325:G:H8    | 27:DA:2325:G:P     | 2.41                     | 0.43              |
| 27:DA:2666:C:H42   | 34:DH:109:PHE:HA   | 1.82                     | 0.43              |
| 27:DA:271(M):G:H2' | 27:DA:271(N):U:C5' | 2.43                     | 0.43              |
| 27:DA:303:U:H6     | 27:DA:303:U:O5'    | 2.00                     | 0.43              |
| 27:DA:35:G:O4'     | 27:DA:454:A:H1'    | 2.17                     | 0.43              |
| 27:DA:464:U:C4     | 27:DA:465:G:C6     | 3.05                     | 0.43              |
| 27:DA:473:G:H5''   | 27:DA:508:G:H22    | 1.81                     | 0.43              |
| 27:DA:481:G:HO2'   | 27:DA:482:A:P      | 2.39                     | 0.43              |
| 27:DA:504:U:O5'    | 27:DA:504:U:C6     | 2.71                     | 0.43              |
| 27:DA:522:G:C5     | 27:DA:523:C:C5     | 3.06                     | 0.43              |
| 27:DA:71:A:C5'     | 27:DA:71:A:H8      | 2.31                     | 0.43              |
| 27:DA:751:A:H2'    | 27:DA:789:A:C2     | 2.52                     | 0.43              |
| 27:DA:800:A:H4'    | 27:DA:801:G:O5'    | 2.17                     | 0.43              |
| 27:DA:867:C:O5'    | 27:DA:867:C:H6     | 2.00                     | 0.43              |
| 27:DA:869:G:N1     | 27:DA:909:A:C6     | 2.86                     | 0.43              |
| 27:DA:910:A:H2'    | 27:DA:911:A:C8     | 2.53                     | 0.43              |
| 27:DA:866:A:C6     | 27:DA:914:C:C6     | 3.06                     | 0.43              |
| 27:DA:985:C:C2'    | 27:DA:986:C:H5'    | 2.48                     | 0.43              |
| 27:DA:986:C:C2     | 27:DA:987:G:C8     | 3.06                     | 0.43              |
| 29:DC:214:VAL:O    | 29:DC:215:THR:C    | 2.56                     | 0.43              |
| 30:DD:35:LYS:NZ    | 30:DD:104:TYR:HB2  | 2.31                     | 0.43              |
| 30:DD:146:GLU:HB3  | 30:DD:153:ALA:HA   | 2.00                     | 0.43              |
| 31:DE:111:ARG:CD   | 31:DE:160:TYR:HE1  | 2.31                     | 0.43              |
| 33:DG:38:VAL:HG13  | 33:DG:93:THR:HA    | 1.99                     | 0.43              |
| 34:DH:19:VAL:HA    | 34:DH:24:VAL:HG12  | 2.00                     | 0.43              |
| 35:DI:102:SER:C    | 35:DI:103:ARG:HG3  | 2.39                     | 0.43              |
| 38:DP:136:GLU:O    | 38:DP:139:LYS:HB2  | 2.18                     | 0.43              |
| 39:DQ:35:VAL:HG23  | 39:DQ:100:GLY:O    | 2.18                     | 0.43              |
| 44:DV:99:ILE:CD1   | 44:DV:99:ILE:N     | 2.77                     | 0.43              |
| 45:DW:11:ARG:CA    | 45:DW:11:ARG:HE    | 2.31                     | 0.43              |
| 46:DX:25:LYS:HZ2   | 46:DX:80:ILE:HD11  | 1.76                     | 0.43              |
| 47:DY:30:VAL:HG12  | 47:DY:31:LEU:N     | 2.32                     | 0.43              |
| 47:DY:3:VAL:O      | 47:DY:4:LYS:C      | 2.55                     | 0.43              |
| 47:DY:46:LYS:HD3   | 47:DY:47:LYS:HZ1   | 1.81                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:DZ:47:PHE:O     | 48:DZ:48:ARG:C    | 2.56                     | 0.43              |
| 48:DZ:68:THR:HG22  | 48:DZ:89:VAL:HA   | 1.99                     | 0.43              |
| 48:DZ:8:TYR:CZ     | 48:DZ:60:LEU:HD12 | 2.53                     | 0.43              |
| 1:AA:1016:A:H2'    | 1:AA:1017:G:C5'   | 2.48                     | 0.43              |
| 1:AA:103:C:C5      | 1:AA:104:G:N7     | 2.86                     | 0.43              |
| 1:AA:1508:G:C4     | 1:AA:1509:C:C6    | 3.05                     | 0.43              |
| 1:AA:411:A:N6      | 1:AA:429:U:C5     | 2.86                     | 0.43              |
| 1:AA:741:G:O2'     | 15:AO:55:GLY:HA3  | 2.18                     | 0.43              |
| 2:AB:22:LYS:HG2    | 2:AB:35:GLU:OE1   | 2.17                     | 0.43              |
| 3:AC:173:VAL:HG12  | 3:AC:173:VAL:O    | 2.17                     | 0.43              |
| 4:AD:205:GLU:O     | 4:AD:206:PHE:C    | 2.57                     | 0.43              |
| 4:AD:22:LYS:HB2    | 4:AD:26:CYS:CB    | 2.45                     | 0.43              |
| 6:AF:18:GLN:CA     | 6:AF:21:LEU:HB2   | 2.43                     | 0.43              |
| 10:AJ:26:ALA:HA    | 10:AJ:29:ARG:HH21 | 1.83                     | 0.43              |
| 10:AJ:81:THR:O     | 10:AJ:85:LEU:HG   | 2.18                     | 0.43              |
| 12:AL:112:LYS:O    | 12:AL:114:ARG:N   | 2.48                     | 0.43              |
| 12:AL:38:ARG:HG2   | 12:AL:39:THR:N    | 2.15                     | 0.43              |
| 27:BA:1158:C:H4'   | 52:B3:31:LEU:O    | 2.18                     | 0.43              |
| 57:B8:36:LYS:HE3   | 57:B8:40:GLU:OE2  | 2.18                     | 0.43              |
| 57:B8:61:LEU:O     | 57:B8:63:PRO:O    | 2.36                     | 0.43              |
| 27:BA:1216:G:O2'   | 27:BA:1217:C:H5'  | 2.18                     | 0.43              |
| 27:BA:1373:A:C2'   | 27:BA:1374:G:H5'  | 2.48                     | 0.43              |
| 27:BA:1412:A:H2'   | 27:BA:1413:G:O4'  | 2.17                     | 0.43              |
| 27:BA:1441:G:N2    | 27:BA:1551:C:C2   | 2.86                     | 0.43              |
| 27:BA:1654:A:OP2   | 40:BR:3:HIS:CD2   | 2.72                     | 0.43              |
| 27:BA:2138:C:O2'   | 27:BA:2139:C:H5'  | 2.17                     | 0.43              |
| 27:BA:2221:G:H2'   | 27:BA:2221:G:N3   | 2.33                     | 0.43              |
| 27:BA:2262:U:N3    | 27:BA:2279:G:C2   | 2.86                     | 0.43              |
| 27:BA:2476:A:C2    | 27:BA:2477:C:H6   | 2.36                     | 0.43              |
| 27:BA:415:A:H3'    | 27:BA:416:C:H6    | 1.81                     | 0.43              |
| 27:BA:527:C:C5     | 27:BA:2779:U:C2'  | 3.01                     | 0.43              |
| 27:BA:55:G:C2      | 27:BA:56:A:N7     | 2.85                     | 0.43              |
| 27:BA:685:A:C8     | 27:BA:774:A:C6    | 3.05                     | 0.43              |
| 27:BA:817:C:O2'    | 27:BA:839:U:H5''  | 2.18                     | 0.43              |
| 27:BA:933:A:C2     | 27:BA:934:G:N7    | 2.86                     | 0.43              |
| 27:BA:941:A:HO2'   | 38:BP:35:HIS:CE1  | 2.36                     | 0.43              |
| 29:BC:200:LYS:O    | 29:BC:202:GLU:N   | 2.51                     | 0.43              |
| 29:BC:24:GLU:CD    | 29:BC:24:GLU:H    | 2.22                     | 0.43              |
| 32:BF:157:VAL:HG13 | 32:BF:178:PRO:HA  | 1.99                     | 0.43              |
| 32:BF:192:LEU:HD21 | 32:BF:194:MET:CE  | 2.48                     | 0.43              |
| 32:BF:202:PHE:O    | 32:BF:205:ARG:N   | 2.51                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:BF:28:ILE:CD1  | 32:BF:28:ILE:O     | 2.64                     | 0.43              |
| 37:BO:23:ARG:HA   | 37:BO:23:ARG:HD3   | 1.81                     | 0.43              |
| 39:BQ:116:GLU:O   | 39:BQ:120:ILE:HG12 | 2.18                     | 0.43              |
| 39:BQ:12:GLN:HE21 | 39:BQ:73:PRO:HD2   | 1.82                     | 0.43              |
| 39:BQ:74:TYR:HB3  | 39:BQ:92:GLY:O     | 2.18                     | 0.43              |
| 41:BS:17:ARG:C    | 41:BS:19:LYS:H     | 2.20                     | 0.43              |
| 41:BS:67:ARG:HG2  | 41:BS:67:ARG:HH11  | 1.82                     | 0.43              |
| 41:BS:99:LYS:H    | 41:BS:99:LYS:HG2   | 1.61                     | 0.43              |
| 42:BT:108:ARG:C   | 42:BT:111:ARG:HG3  | 2.38                     | 0.43              |
| 42:BT:56:GLY:O    | 42:BT:59:THR:CG2   | 2.66                     | 0.43              |
| 44:BV:4:ILE:HB    | 44:BV:39:LEU:O     | 2.17                     | 0.43              |
| 46:BX:40:LYS:HG3  | 46:BX:51:VAL:HB    | 1.99                     | 0.43              |
| 27:BA:329:G:H1    | 47:BY:19:LYS:HZ1   | 1.64                     | 0.43              |
| 47:BY:7:VAL:HG12  | 47:BY:83:THR:HG21  | 2.00                     | 0.43              |
| 47:BY:84:ARG:HH11 | 47:BY:97:ARG:HA    | 1.83                     | 0.43              |
| 48:BZ:140:VAL:CG2 | 48:BZ:143:LEU:HD23 | 2.41                     | 0.43              |
| 48:BZ:149:LEU:O   | 48:BZ:170:ILE:CD1  | 2.65                     | 0.43              |
| 48:BZ:26:VAL:HG23 | 48:BZ:35:LYS:HA    | 1.99                     | 0.43              |
| 39:BQ:141:GLN:OE1 | 48:BZ:71:ARG:O     | 2.36                     | 0.43              |
| 1:CA:101:A:H2'    | 1:CA:102:G:C5'     | 2.48                     | 0.43              |
| 1:CA:1057:G:O2'   | 1:CA:1058:G:H5'    | 2.18                     | 0.43              |
| 1:CA:1064:G:O2'   | 1:CA:1065:U:O5'    | 2.25                     | 0.43              |
| 1:CA:1117:G:H4'   | 9:CI:104:ARG:NH1   | 2.33                     | 0.43              |
| 1:CA:1116:C:C3'   | 1:CA:1117:G:H5''   | 2.48                     | 0.43              |
| 1:CA:1193:G:C5    | 1:CA:1194:U:C5     | 3.06                     | 0.43              |
| 1:CA:1459:C:H4'   | 20:CT:24:LEU:HD21  | 2.00                     | 0.43              |
| 1:CA:1466:C:C5    | 1:CA:1467:G:N7     | 2.87                     | 0.43              |
| 1:CA:338:A:H2'    | 1:CA:339:C:C6      | 2.52                     | 0.43              |
| 1:CA:545:C:OP1    | 4:CD:61:LYS:NZ     | 2.51                     | 0.43              |
| 1:CA:560:U:C5'    | 1:CA:566:G:N2      | 2.81                     | 0.43              |
| 1:CA:628:G:C2'    | 1:CA:629:G:H5'     | 2.48                     | 0.43              |
| 2:CB:171:ALA:C    | 2:CB:173:ALA:N     | 2.70                     | 0.43              |
| 2:CB:77:ALA:CB    | 2:CB:211:ILE:HG21  | 2.48                     | 0.43              |
| 6:CF:22:GLU:OE1   | 6:CF:82:ARG:NH2    | 2.51                     | 0.43              |
| 6:CF:91:VAL:O     | 6:CF:92:LYS:C      | 2.56                     | 0.43              |
| 7:CG:57:GLU:O     | 7:CG:57:GLU:HG3    | 2.17                     | 0.43              |
| 8:CH:109:ILE:CG1  | 8:CH:110:ALA:H     | 2.22                     | 0.43              |
| 8:CH:20:TYR:HD1   | 8:CH:65:TYR:CD2    | 2.36                     | 0.43              |
| 12:CL:23:ALA:O    | 12:CL:24:LEU:HD22  | 2.18                     | 0.43              |
| 1:CA:948:C:C5     | 13:CM:106:ASN:ND2  | 2.87                     | 0.43              |
| 13:CM:7:VAL:HG12  | 13:CM:7:VAL:O      | 2.17                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CP:21:VAL:O     | 16:CP:21:VAL:CG1   | 2.65                     | 0.43              |
| 25:CY:54:U:C6      | 25:CY:57:A:N7      | 2.86                     | 0.43              |
| 50:D1:45:ASN:CG    | 50:D1:45:ASN:O     | 2.56                     | 0.43              |
| 27:DA:850:C:O2'    | 52:D3:46:ASN:ND2   | 2.51                     | 0.43              |
| 54:D5:45:VAL:HG22  | 54:D5:51:TYR:CD2   | 2.53                     | 0.43              |
| 55:D6:8:LYS:CG     | 55:D6:8:LYS:O      | 2.66                     | 0.43              |
| 27:DA:1311:G:C4    | 56:D7:47:ARG:NH2   | 2.86                     | 0.43              |
| 27:DA:108:U:C2     | 27:DA:109:G:C8     | 3.06                     | 0.43              |
| 27:DA:1000:A:C5    | 27:DA:1155:A:C5    | 3.06                     | 0.43              |
| 27:DA:1204:A:C5    | 27:DA:1206:G:N1    | 2.86                     | 0.43              |
| 27:DA:1423:G:N2    | 27:DA:1576:U:O2    | 2.50                     | 0.43              |
| 27:DA:147:U:O2'    | 27:DA:148:C:H5'    | 2.17                     | 0.43              |
| 27:DA:1741:A:O2'   | 27:DA:1742:G:O4'   | 2.36                     | 0.43              |
| 27:DA:1829:A:N3    | 30:DD:15:PHE:CZ    | 2.85                     | 0.43              |
| 27:DA:1911:U:C2'   | 27:DA:1912:A:H5''  | 2.48                     | 0.43              |
| 27:DA:1679:U:H1'   | 27:DA:1989:G:N2    | 2.33                     | 0.43              |
| 27:DA:2470:G:C4    | 27:DA:2471:C:C5    | 3.06                     | 0.43              |
| 27:DA:2522:U:H2'   | 27:DA:2523:G:H5'   | 2.00                     | 0.43              |
| 27:DA:2653:U:H3'   | 27:DA:2654:A:C8    | 2.53                     | 0.43              |
| 27:DA:2803:C:H2'   | 27:DA:2804:C:C6    | 2.53                     | 0.43              |
| 27:DA:2848:G:N3    | 27:DA:2867:G:C2    | 2.86                     | 0.43              |
| 27:DA:35:G:C6      | 27:DA:36:G:N7      | 2.85                     | 0.43              |
| 27:DA:51:G:N3      | 27:DA:119:A:H2     | 2.15                     | 0.43              |
| 27:DA:534:U:O2'    | 43:DU:46:ALA:HA    | 2.18                     | 0.43              |
| 27:DA:630:G:N2     | 27:DA:634:C:N3     | 2.66                     | 0.43              |
| 27:DA:693:C:H2'    | 27:DA:694:U:O4'    | 2.18                     | 0.43              |
| 27:DA:826:U:C5     | 27:DA:828:U:H1'    | 2.53                     | 0.43              |
| 27:DA:968:G:C6     | 27:DA:969:U:C4     | 3.05                     | 0.43              |
| 27:DA:977:G:C2     | 27:DA:978:G:C8     | 3.06                     | 0.43              |
| 29:DC:86:ALA:HB3   | 29:DC:94:VAL:HG11  | 2.00                     | 0.43              |
| 30:DD:123:ALA:CB   | 30:DD:131:LEU:HD11 | 2.48                     | 0.43              |
| 30:DD:141:VAL:HG23 | 30:DD:142:VAL:N    | 2.32                     | 0.43              |
| 30:DD:182:LEU:HB2  | 30:DD:271:ILE:HG13 | 1.99                     | 0.43              |
| 30:DD:25:THR:O     | 30:DD:27:THR:HG22  | 2.18                     | 0.43              |
| 27:DA:1567:A:C5'   | 30:DD:58:HIS:CD2   | 2.98                     | 0.43              |
| 27:DA:1257:C:H4'   | 32:DF:83:PHE:CE2   | 2.53                     | 0.43              |
| 32:DF:96:ASP:OD2   | 32:DF:98:SER:OG    | 2.30                     | 0.43              |
| 33:DG:9:ARG:O      | 33:DG:11:TYR:N     | 2.51                     | 0.43              |
| 34:DH:107:VAL:O    | 34:DH:109:PHE:N    | 2.44                     | 0.43              |
| 35:DI:76:THR:HG22  | 35:DI:139:GLN:HB3  | 2.00                     | 0.43              |
| 37:DO:64:ARG:O     | 37:DO:82:ASN:HA    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 38:DP:58:THR:C   | 38:DP:60:MET:H    | 2.22                     | 0.43              |
| 39:DQ:18:LYS:HB2 | 39:DQ:98:LYS:HZ1  | 1.83                     | 0.43              |
| 44:DV:64:HIS:ND1 | 44:DV:92:THR:HG23 | 2.33                     | 0.43              |
| 47:DY:16:ALA:HA  | 47:DY:21:LYS:HD3  | 1.99                     | 0.43              |
| 1:AA:1010:G:N2   | 1:AA:1020:U:H1'   | 2.33                     | 0.43              |
| 1:AA:1047:G:O2'  | 1:AA:1048:G:H5'   | 2.18                     | 0.43              |
| 1:AA:1403:C:H2'  | 1:AA:1404:C:C6    | 2.53                     | 0.43              |
| 1:AA:1509:C:O2'  | 1:AA:1510:U:H5'   | 2.18                     | 0.43              |
| 1:AA:374:A:H2'   | 1:AA:375:U:C6     | 2.54                     | 0.43              |
| 1:AA:392:G:H5'   | 16:AP:13:HIS:NE2  | 2.32                     | 0.43              |
| 1:AA:417:C:O2'   | 1:AA:418:C:H5'    | 2.18                     | 0.43              |
| 1:AA:448:A:C2    | 1:AA:449:C:C4     | 3.07                     | 0.43              |
| 1:AA:576:G:C2    | 1:AA:881:G:H4'    | 2.53                     | 0.43              |
| 1:AA:695:A:H2'   | 1:AA:696:A:C8     | 2.53                     | 0.43              |
| 1:AA:877:C:H5''  | 8:AH:88:LYS:HD3   | 2.00                     | 0.43              |
| 1:AA:937:A:C2    | 1:AA:1379:G:C6    | 3.06                     | 0.43              |
| 1:AA:944:G:H1'   | 1:AA:1340:A:H2    | 1.82                     | 0.43              |
| 2:AB:9:GLU:O     | 2:AB:11:LEU:N     | 2.51                     | 0.43              |
| 2:AB:152:PHE:C   | 2:AB:154:LEU:N    | 2.69                     | 0.43              |
| 2:AB:73:THR:O    | 2:AB:74:LYS:C     | 2.56                     | 0.43              |
| 4:AD:138:TYR:CD2 | 4:AD:138:TYR:C    | 2.91                     | 0.43              |
| 7:AG:52:GLU:O    | 7:AG:54:THR:N     | 2.51                     | 0.43              |
| 7:AG:92:SER:HB2  | 7:AG:94:ARG:HH21  | 1.83                     | 0.43              |
| 8:AH:102:ARG:HD2 | 8:AH:105:ARG:NH1  | 2.33                     | 0.43              |
| 8:AH:124:ALA:CA  | 8:AH:129:VAL:HG22 | 2.48                     | 0.43              |
| 8:AH:75:ARG:HE   | 8:AH:75:ARG:HB2   | 1.50                     | 0.43              |
| 9:AI:76:ALA:O    | 9:AI:79:LEU:HB3   | 2.19                     | 0.43              |
| 10:AJ:13:HIS:O   | 10:AJ:17:ASP:HB2  | 2.18                     | 0.43              |
| 10:AJ:45:ARG:HG3 | 10:AJ:45:ARG:HH11 | 1.83                     | 0.43              |
| 10:AJ:51:ARG:HG3 | 10:AJ:60:ARG:C    | 2.38                     | 0.43              |
| 11:AK:62:GLN:O   | 11:AK:63:LEU:C    | 2.57                     | 0.43              |
| 12:AL:15:VAL:O   | 12:AL:16:ARG:HB3  | 2.18                     | 0.43              |
| 12:AL:2:PRO:HA   | 12:AL:6:GLN:HE21  | 1.83                     | 0.43              |
| 13:AM:12:ASN:HB3 | 13:AM:46:LYS:HE2  | 1.99                     | 0.43              |
| 13:AM:81:LEU:H   | 13:AM:81:LEU:HD12 | 1.84                     | 0.43              |
| 13:AM:81:LEU:N   | 13:AM:81:LEU:HD12 | 2.33                     | 0.43              |
| 1:AA:254:G:OP1   | 17:AQ:67:LYS:O    | 2.36                     | 0.43              |
| 19:AS:4:SER:O    | 19:AS:5:LEU:CB    | 2.60                     | 0.43              |
| 21:AU:13:ILE:CG1 | 21:AU:22:ARG:HE   | 2.30                     | 0.43              |
| 22:AV:9:G:N2     | 23:AW:34:U:N3     | 2.66                     | 0.43              |
| 23:AW:16:C:H5'   | 23:AW:58:A:N1     | 2.32                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:B0:71:ASP:HA   | 49:B0:77:ARG:HA   | 2.00                     | 0.43              |
| 51:B2:10:LEU:HA   | 51:B2:10:LEU:HD23 | 1.88                     | 0.43              |
| 51:B2:36:ARG:C    | 51:B2:38:GLN:H    | 2.21                     | 0.43              |
| 52:B3:4:LEU:HA    | 52:B3:4:LEU:HD23  | 1.86                     | 0.43              |
| 54:B5:16:ARG:NH1  | 54:B5:17:ASP:OD1  | 2.51                     | 0.43              |
| 27:BA:1007:C:OP1  | 36:BN:35:ARG:NH1  | 2.50                     | 0.43              |
| 27:BA:1050:A:O2'  | 27:BA:1051:G:C8   | 2.61                     | 0.43              |
| 27:BA:1167:U:H2'  | 27:BA:1168:G:H8   | 1.83                     | 0.43              |
| 27:BA:1178:C:C6   | 27:BA:1179:C:H5   | 2.34                     | 0.43              |
| 27:BA:1391:U:O2   | 27:BA:1393:A:C8   | 2.71                     | 0.43              |
| 27:BA:1468:C:O2   | 27:BA:1468:C:H2'  | 2.17                     | 0.43              |
| 27:BA:1523:U:H2'  | 27:BA:1524:G:O4'  | 2.19                     | 0.43              |
| 27:BA:1556:C:HO2' | 27:BA:1557:C:H6   | 1.66                     | 0.43              |
| 27:BA:118:A:N3    | 27:BA:178:G:H1'   | 2.33                     | 0.43              |
| 27:BA:1955:U:H2'  | 27:BA:1955:U:O2   | 2.19                     | 0.43              |
| 27:BA:2047:U:C2'  | 27:BA:2048:G:H5'' | 2.48                     | 0.43              |
| 27:BA:2145:C:H4'  | 27:BA:2146:C:OP2  | 2.18                     | 0.43              |
| 27:BA:2171:A:O2'  | 27:BA:2172:U:H6   | 2.01                     | 0.43              |
| 27:BA:2192:G:C2   | 27:BA:2193:G:C8   | 3.06                     | 0.43              |
| 27:BA:2439:A:C5'  | 27:BA:2439:A:C8   | 2.94                     | 0.43              |
| 27:BA:2580:U:C5   | 27:BA:2581:G:C6   | 3.06                     | 0.43              |
| 27:BA:2692:C:O2'  | 27:BA:2693:A:H5'  | 2.19                     | 0.43              |
| 27:BA:2716:U:O2'  | 27:BA:2717:G:H5'  | 2.18                     | 0.43              |
| 27:BA:2759:G:C2   | 27:BA:2760:C:C2   | 3.05                     | 0.43              |
| 27:BA:2761:G:N2   | 27:BA:2762:G:H1'  | 2.34                     | 0.43              |
| 27:BA:2805:G:C2   | 27:BA:2807:G:C5   | 3.06                     | 0.43              |
| 27:BA:463:G:N2    | 27:BA:467:G:C4    | 2.86                     | 0.43              |
| 27:BA:728:G:H4'   | 30:BD:13:ARG:CD   | 2.48                     | 0.43              |
| 28:BB:23:G:N2     | 28:BB:61:G:C4     | 2.86                     | 0.43              |
| 28:BB:87:G:H2'    | 28:BB:88:C:H5''   | 2.00                     | 0.43              |
| 31:BE:39:PRO:HG3  | 31:BE:45:THR:OG1  | 2.18                     | 0.43              |
| 32:BF:110:LEU:CD1 | 32:BF:110:LEU:C   | 2.87                     | 0.43              |
| 34:BH:23:ARG:N    | 34:BH:23:ARG:HD3  | 2.33                     | 0.43              |
| 35:BI:3:VAL:HA    | 35:BI:39:ALA:CB   | 2.42                     | 0.43              |
| 37:BO:23:ARG:HG2  | 37:BO:23:ARG:NH1  | 2.33                     | 0.43              |
| 37:BO:23:ARG:CG   | 37:BO:23:ARG:HH11 | 2.31                     | 0.43              |
| 37:BO:7:TYR:O     | 37:BO:8:LEU:HD13  | 2.18                     | 0.43              |
| 44:BV:19:LYS:NZ   | 44:BV:20:LEU:H    | 2.16                     | 0.43              |
| 44:BV:47:VAL:CB   | 44:BV:49:THR:O    | 2.63                     | 0.43              |
| 45:BW:15:ARG:O    | 45:BW:19:LEU:HD22 | 2.19                     | 0.43              |
| 46:BX:32:PRO:HA   | 46:BX:77:LYS:CB   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 48:BZ:15:SER:O    | 48:BZ:18:ARG:HB2 | 2.18                     | 0.43              |
| 1:CA:61:G:C6      | 1:CA:107:G:C2    | 3.07                     | 0.43              |
| 1:CA:1185:G:C4    | 1:CA:1186:G:C8   | 3.07                     | 0.43              |
| 1:CA:1246:C:H6    | 1:CA:1246:C:O5'  | 2.01                     | 0.43              |
| 1:CA:1288:A:H2'   | 1:CA:1289:A:O4'  | 2.17                     | 0.43              |
| 1:CA:1238:A:N7    | 1:CA:1303:C:O4'  | 2.52                     | 0.43              |
| 1:CA:346:G:C5'    | 42:DT:41:ARG:NH2 | 2.82                     | 0.43              |
| 1:CA:501:C:H2'    | 1:CA:502:G:H8    | 1.80                     | 0.43              |
| 1:CA:519:C:H2'    | 1:CA:520:A:O4'   | 2.18                     | 0.43              |
| 1:CA:577:G:C4     | 1:CA:578:C:C5    | 3.06                     | 0.43              |
| 1:CA:623:C:N3     | 1:CA:624:C:C5    | 2.86                     | 0.43              |
| 1:CA:775:G:H2'    | 1:CA:776:G:O4'   | 2.18                     | 0.43              |
| 1:CA:841:U:H3'    | 1:CA:848:C:C6    | 2.53                     | 0.43              |
| 3:CC:179:ARG:O    | 3:CC:181:ASN:N   | 2.52                     | 0.43              |
| 4:CD:25:ARG:C     | 4:CD:27:TYR:H    | 2.21                     | 0.43              |
| 4:CD:73:ARG:HG3   | 4:CD:77:ASN:OD1  | 2.18                     | 0.43              |
| 5:CE:105:VAL:CB   | 5:CE:106:PRO:CD  | 2.96                     | 0.43              |
| 5:CE:33:VAL:HA    | 5:CE:43:LEU:HD12 | 1.98                     | 0.43              |
| 6:CF:50:TYR:CE2   | 6:CF:52:ILE:HD11 | 2.53                     | 0.43              |
| 8:CH:127:LEU:HD22 | 8:CH:127:LEU:HA  | 1.79                     | 0.43              |
| 10:CJ:54:PHE:CE1  | 10:CJ:55:LYS:HE3 | 2.53                     | 0.43              |
| 10:CJ:85:LEU:O    | 10:CJ:87:THR:O   | 2.36                     | 0.43              |
| 12:CL:81:LEU:O    | 12:CL:97:ILE:HA  | 2.17                     | 0.43              |
| 15:CO:7:GLU:O     | 15:CO:10:LYS:HE3 | 2.19                     | 0.43              |
| 19:CS:20:LEU:CA   | 19:CS:23:ASN:HB3 | 2.49                     | 0.43              |
| 19:CS:61:TYR:O    | 19:CS:62:ILE:CB  | 2.65                     | 0.43              |
| 20:CT:50:GLU:O    | 20:CT:54:LYS:CB  | 2.66                     | 0.43              |
| 25:CY:27:C:H42    | 25:CY:41:G:H1    | 1.64                     | 0.43              |
| 50:D1:23:LYS:HE2  | 50:D1:28:GLY:CA  | 2.49                     | 0.43              |
| 52:D3:7:LYS:HG3   | 52:D3:34:GLU:CG  | 2.41                     | 0.43              |
| 57:D8:23:VAL:HG12 | 57:D8:46:ARG:HB3 | 2.00                     | 0.43              |
| 57:D8:50:LEU:O    | 57:D8:51:ALA:CB  | 2.66                     | 0.43              |
| 27:DA:1274:A:H2   | 27:DA:1644:C:O2  | 2.00                     | 0.43              |
| 27:DA:1301:A:C4   | 27:DA:1303:G:N7  | 2.87                     | 0.43              |
| 27:DA:133:C:N3    | 27:DA:146:G:N2   | 2.49                     | 0.43              |
| 27:DA:1857:G:O2'  | 27:DA:1885:A:N6  | 2.51                     | 0.43              |
| 27:DA:1924:C:O2'  | 27:DA:1925:C:H5' | 2.17                     | 0.43              |
| 1:CA:1418:A:H1'   | 27:DA:1959:G:H4' | 2.00                     | 0.43              |
| 27:DA:2294:C:H2'  | 27:DA:2294:C:O2  | 2.18                     | 0.43              |
| 27:DA:2374:C:H2'  | 27:DA:2375:G:O4' | 2.18                     | 0.43              |
| 27:DA:2472:G:H1   | 27:DA:2477:C:P   | 2.40                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2528:U:H2'   | 27:DA:2530:A:O5'   | 2.18                     | 0.43              |
| 27:DA:2681:C:C5    | 27:DA:2724:C:N4    | 2.87                     | 0.43              |
| 27:DA:271(F):C:O5' | 27:DA:271(F):C:H6  | 2.01                     | 0.43              |
| 27:DA:271(I):G:H2' | 27:DA:271(J):C:H1' | 2.00                     | 0.43              |
| 27:DA:2776:A:C5'   | 27:DA:2778:A:OP1   | 2.67                     | 0.43              |
| 27:DA:358:U:H6     | 27:DA:358:U:OP2    | 2.00                     | 0.43              |
| 27:DA:552:G:H2'    | 27:DA:553:G:H5'    | 1.98                     | 0.43              |
| 29:DC:82:LYS:O     | 29:DC:86:ALA:HB3   | 2.18                     | 0.43              |
| 30:DD:28:GLU:HB2   | 30:DD:29:PRO:HD3   | 2.00                     | 0.43              |
| 33:DG:75:LYS:HB3   | 33:DG:76:SER:H     | 1.57                     | 0.43              |
| 37:DO:66:LYS:HD3   | 37:DO:79:PHE:C     | 2.38                     | 0.43              |
| 37:DO:77:ILE:HD11  | 42:DT:72:VAL:HG13  | 1.99                     | 0.43              |
| 38:DP:30:THR:HG22  | 38:DP:31:ALA:N     | 2.33                     | 0.43              |
| 38:DP:23:PRO:CB    | 38:DP:33:ARG:NE    | 2.80                     | 0.43              |
| 40:DR:20:LEU:HG    | 40:DR:21:TYR:N     | 2.32                     | 0.43              |
| 42:DT:65:LYS:NZ    | 42:DT:66:VAL:N     | 2.31                     | 0.43              |
| 43:DU:62:ILE:O     | 43:DU:63:VAL:C     | 2.55                     | 0.43              |
| 44:DV:49:THR:O     | 44:DV:50:PRO:C     | 2.56                     | 0.43              |
| 46:DX:41:ASN:N     | 46:DX:41:ASN:ND2   | 2.67                     | 0.43              |
| 46:DX:57:LEU:HD13  | 46:DX:78:LYS:HG2   | 1.96                     | 0.43              |
| 1:AA:1047:G:H1     | 1:AA:1210:C:N4     | 2.16                     | 0.43              |
| 1:AA:1066:C:H5''   | 1:AA:1066:C:C6     | 2.53                     | 0.43              |
| 1:AA:1405:G:C2'    | 1:AA:1406:U:O5'    | 2.67                     | 0.43              |
| 1:AA:1495:U:H2'    | 1:AA:1496:C:H6     | 1.84                     | 0.43              |
| 1:AA:176:C:C2      | 1:AA:177:C:C5      | 3.05                     | 0.43              |
| 1:AA:18:C:H2'      | 1:AA:19:C:O4'      | 2.18                     | 0.43              |
| 1:AA:335:C:O2'     | 1:AA:336:C:H5'     | 2.18                     | 0.43              |
| 1:AA:355:C:H2'     | 1:AA:356:A:O5'     | 2.18                     | 0.43              |
| 1:AA:600:C:N3      | 1:AA:639:G:C2      | 2.86                     | 0.43              |
| 1:AA:859:A:H2'     | 1:AA:860:A:H8      | 1.84                     | 0.43              |
| 2:AB:166:ASP:O     | 2:AB:167:PRO:C     | 2.56                     | 0.43              |
| 2:AB:21:ARG:C      | 2:AB:23:ARG:H      | 2.21                     | 0.43              |
| 3:AC:166:GLU:HA    | 3:AC:166:GLU:OE2   | 2.18                     | 0.43              |
| 3:AC:172:ARG:HB3   | 3:AC:174:PRO:HD3   | 1.99                     | 0.43              |
| 3:AC:29:TYR:HE2    | 3:AC:33:LEU:HD13   | 1.83                     | 0.43              |
| 3:AC:60:ALA:O      | 3:AC:61:ALA:HB2    | 2.18                     | 0.43              |
| 5:AE:96:PRO:HA     | 5:AE:117:ASP:OD2   | 2.18                     | 0.43              |
| 6:AF:80:ARG:C      | 6:AF:82:ARG:N      | 2.71                     | 0.43              |
| 7:AG:120:ILE:O     | 7:AG:124:LEU:HG    | 2.18                     | 0.43              |
| 1:AA:1380:U:O4     | 7:AG:3:ARG:HA      | 2.18                     | 0.43              |
| 13:AM:48:LEU:N     | 13:AM:48:LEU:HD23  | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:AM:93:ARG:HA   | 13:AM:93:ARG:HE   | 1.83                     | 0.43              |
| 1:AA:1060:C:C5'   | 14:AN:45:ARG:NH2  | 2.78                     | 0.43              |
| 23:AW:65:U:O2'    | 23:AW:66:A:H5'    | 2.18                     | 0.43              |
| 23:AW:8:U:HO2'    | 23:AW:44:A:H2     | 1.65                     | 0.43              |
| 25:AY:14:A:H1'    | 25:AY:21:A:N1     | 2.33                     | 0.43              |
| 7:AG:86:GLN:NE2   | 25:AY:30:A:C2     | 2.85                     | 0.43              |
| 50:B1:6:GLU:C     | 50:B1:7:ILE:HD12  | 2.38                     | 0.43              |
| 27:BA:1598:C:H5'  | 46:BX:36:LYS:HG3  | 1.99                     | 0.43              |
| 27:BA:1686:C:H2'  | 27:BA:1687:G:H5'  | 2.00                     | 0.43              |
| 27:BA:1703:G:N2   | 27:BA:1704:G:C4   | 2.87                     | 0.43              |
| 27:BA:2056:G:H1   | 54:B5:4:HIS:CD2   | 2.36                     | 0.43              |
| 27:BA:2072:G:C5   | 27:BA:2073:C:C5   | 3.07                     | 0.43              |
| 27:BA:2088:G:H2'  | 27:BA:2089:U:H6   | 1.81                     | 0.43              |
| 27:BA:2163:C:C2'  | 27:BA:2164:C:H5'  | 2.48                     | 0.43              |
| 27:BA:2264:C:N4   | 27:BA:2265:U:O4   | 2.51                     | 0.43              |
| 27:BA:2353:G:C5   | 27:BA:2365:G:N2   | 2.85                     | 0.43              |
| 27:BA:2460:U:C4   | 27:BA:2461:C:C5   | 3.06                     | 0.43              |
| 27:BA:2591:C:H2'  | 27:BA:2592:G:H8   | 1.83                     | 0.43              |
| 27:BA:2673:G:O2'  | 27:BA:2674:G:H5'  | 2.18                     | 0.43              |
| 27:BA:2766:G:C2   | 27:BA:2767:C:C6   | 3.06                     | 0.43              |
| 27:BA:2788:C:H4'  | 27:BA:2810:A:O4'  | 2.18                     | 0.43              |
| 27:BA:2842:G:C4   | 27:BA:2876:G:N2   | 2.86                     | 0.43              |
| 27:BA:481:G:HO2'  | 27:BA:482:A:P     | 2.38                     | 0.43              |
| 27:BA:846:C:C2    | 27:BA:930:U:C4    | 3.06                     | 0.43              |
| 30:BD:60:ARG:CD   | 30:BD:86:PRO:CG   | 2.84                     | 0.43              |
| 27:BA:2772:C:H5'  | 31:BE:168:MET:HE2 | 1.99                     | 0.43              |
| 31:BE:35:GLN:NE2  | 31:BE:37:ARG:NH1  | 2.66                     | 0.43              |
| 35:BI:37:VAL:HG12 | 35:BI:38:LEU:CD1  | 2.48                     | 0.43              |
| 38:BP:85:LEU:HA   | 38:BP:88:LEU:HD22 | 2.01                     | 0.43              |
| 40:BR:62:ALA:O    | 40:BR:63:ARG:C    | 2.56                     | 0.43              |
| 42:BT:106:SER:C   | 42:BT:107:ASP:CG  | 2.76                     | 0.43              |
| 42:BT:13:ARG:O    | 42:BT:15:VAL:HG12 | 2.18                     | 0.43              |
| 36:BN:40:PRO:HB3  | 43:BU:68:ALA:HB2  | 1.99                     | 0.43              |
| 48:BZ:165:SER:CB  | 48:BZ:166:PRO:C   | 2.87                     | 0.43              |
| 48:BZ:23:LEU:O    | 48:BZ:37:TYR:HA   | 2.17                     | 0.43              |
| 1:CA:1038:C:H2'   | 1:CA:1039:C:C5    | 2.53                     | 0.43              |
| 1:CA:103:C:P      | 20:CT:17:ARG:HH12 | 2.41                     | 0.43              |
| 1:CA:1126:U:O2'   | 1:CA:1127:G:H5'   | 2.18                     | 0.43              |
| 1:CA:1356:G:H2'   | 1:CA:1357:A:C8    | 2.53                     | 0.43              |
| 1:CA:1419:G:C4    | 1:CA:1420:C:C5    | 3.07                     | 0.43              |
| 1:CA:1494:G:OP2   | 1:CA:1494:G:C8    | 2.72                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:185:A:C6      | 1:CA:186:C:C4      | 3.07                     | 0.43              |
| 1:CA:320:C:O2'     | 1:CA:1435:G:H1'    | 2.18                     | 0.43              |
| 1:CA:327:A:O3'     | 1:CA:328:C:C4'     | 2.66                     | 0.43              |
| 1:CA:353:A:C8      | 1:CA:353:A:H5'     | 2.52                     | 0.43              |
| 1:CA:995:C:O2'     | 1:CA:996:A:P       | 2.77                     | 0.43              |
| 2:CB:185:ILE:HA    | 2:CB:199:TYR:O     | 2.18                     | 0.43              |
| 3:CC:79:ARG:C      | 3:CC:81:GLY:N      | 2.71                     | 0.43              |
| 3:CC:84:ILE:HA     | 3:CC:87:LEU:CD1    | 2.48                     | 0.43              |
| 4:CD:8:VAL:C       | 4:CD:10:ARG:H      | 2.18                     | 0.43              |
| 4:CD:113:SER:O     | 4:CD:114:ARG:C     | 2.57                     | 0.43              |
| 4:CD:144:ASP:OD1   | 4:CD:144:ASP:N     | 2.51                     | 0.43              |
| 6:CF:22:GLU:HA     | 6:CF:22:GLU:OE2    | 2.18                     | 0.43              |
| 1:CA:1375:A:H4'    | 7:CG:29:LYS:NZ     | 2.34                     | 0.43              |
| 8:CH:30:ARG:O      | 8:CH:33:GLU:N      | 2.52                     | 0.43              |
| 8:CH:49:GLU:OE1    | 8:CH:62:TYR:OH     | 2.35                     | 0.43              |
| 8:CH:44:PHE:HA     | 8:CH:79:VAL:HG11   | 2.00                     | 0.43              |
| 10:CJ:71:LEU:O     | 10:CJ:72:VAL:HG23  | 2.18                     | 0.43              |
| 11:CK:32:ILE:HG13  | 11:CK:40:ILE:HB    | 2.00                     | 0.43              |
| 11:CK:67:ASP:O     | 11:CK:68:ALA:C     | 2.57                     | 0.43              |
| 12:CL:32:GLY:HA3   | 12:CL:57:LEU:CD1   | 2.47                     | 0.43              |
| 1:CA:880:C:C6      | 12:CL:6:GLN:OE1    | 2.71                     | 0.43              |
| 13:CM:16:ASP:CB    | 13:CM:31:LYS:HE2   | 2.48                     | 0.43              |
| 13:CM:69:GLU:HA    | 13:CM:72:ALA:H     | 1.80                     | 0.43              |
| 16:CP:58:TYR:C     | 16:CP:60:LEU:N     | 2.72                     | 0.43              |
| 1:CA:130:A:C8      | 17:CQ:63:ARG:HG3   | 2.52                     | 0.43              |
| 17:CQ:64:PRO:CA    | 17:CQ:70:ARG:HG2   | 2.48                     | 0.43              |
| 20:CT:65:LYS:C     | 20:CT:67:ALA:H     | 2.22                     | 0.43              |
| 23:CW:30:A:C2'     | 23:CW:31:U:C5'     | 2.95                     | 0.43              |
| 25:CY:37:U:H2'     | 25:CY:38:U:C4'     | 2.48                     | 0.43              |
| 50:D1:82:LEU:HD22  | 50:D1:82:LEU:N     | 2.34                     | 0.43              |
| 51:D2:18:PRO:CG    | 51:D2:19:VAL:H     | 2.28                     | 0.43              |
| 54:D5:55:ARG:HD2   | 54:D5:56:LYS:H     | 1.84                     | 0.43              |
| 57:D8:64:TYR:CD1   | 57:D8:64:TYR:N     | 2.86                     | 0.43              |
| 27:DA:1053:C:O2    | 27:DA:1053:C:H2'   | 2.19                     | 0.43              |
| 27:DA:1019:U:N3    | 27:DA:1142(A):A:N6 | 2.55                     | 0.43              |
| 27:DA:1169:G:O5'   | 27:DA:1169:G:H8    | 2.02                     | 0.43              |
| 27:DA:1208:C:N3    | 27:DA:1239:G:C2    | 2.86                     | 0.43              |
| 27:DA:1247:A:C5    | 27:DA:1249:U:C5    | 3.06                     | 0.43              |
| 27:DA:127:A:H5''   | 27:DA:128:C:C6     | 2.53                     | 0.43              |
| 27:DA:142(A):C:O2' | 27:DA:143:G:H5'    | 2.19                     | 0.43              |
| 27:DA:1469:A:H2'   | 27:DA:1470:G:C8    | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DA:1525:G:H2'  | 27:DA:1526:G:H8   | 1.83                     | 0.43              |
| 27:DA:1429:G:H1'  | 27:DA:1568:G:N3   | 2.33                     | 0.43              |
| 27:DA:1300:U:C6   | 27:DA:1626:G:C6   | 3.06                     | 0.43              |
| 27:DA:1754:C:OP1  | 42:DT:95:ARG:HB2  | 2.19                     | 0.43              |
| 27:DA:1826:G:C6   | 27:DA:1827:C:C4   | 3.06                     | 0.43              |
| 27:DA:1914:C:H2'  | 27:DA:1915:U:H6   | 1.83                     | 0.43              |
| 27:DA:2056:G:C2'  | 27:DA:2057:A:H5'  | 2.49                     | 0.43              |
| 27:DA:2063:C:O2'  | 27:DA:2064:C:H5'  | 2.18                     | 0.43              |
| 27:DA:2263:C:O2'  | 27:DA:2264:C:H5'  | 2.18                     | 0.43              |
| 27:DA:2297:C:C2   | 27:DA:2321:G:N2   | 2.81                     | 0.43              |
| 27:DA:2308:G:C2'  | 27:DA:2309:A:C8   | 2.97                     | 0.43              |
| 27:DA:2320:A:N3   | 27:DA:2320:A:H2'  | 2.32                     | 0.43              |
| 27:DA:2523:G:H5'  | 27:DA:2523:G:C8   | 2.46                     | 0.43              |
| 27:DA:2597:G:C6   | 27:DA:2598:A:N6   | 2.86                     | 0.43              |
| 27:DA:469:G:C6    | 56:D7:39:ARG:NH1  | 2.87                     | 0.43              |
| 28:DB:66:A:O2'    | 28:DB:67:G:OP2    | 2.33                     | 0.43              |
| 28:DB:87:G:N1     | 28:DB:91:C:N4     | 2.65                     | 0.43              |
| 30:DD:39:LYS:HD2  | 30:DD:60:ARG:HD2  | 1.99                     | 0.43              |
| 31:DE:25:VAL:HG12 | 31:DE:26:ILE:N    | 2.33                     | 0.43              |
| 31:DE:61:ARG:CB   | 31:DE:62:PRO:CD   | 2.97                     | 0.43              |
| 32:DF:135:LYS:HE3 | 32:DF:137:LYS:HG3 | 2.00                     | 0.43              |
| 27:DA:674:G:H5''  | 32:DF:76:GLY:N    | 2.33                     | 0.43              |
| 33:DG:9:ARG:O     | 33:DG:10:LYS:C    | 2.56                     | 0.43              |
| 27:DA:1006:C:O2   | 36:DN:106:MET:HG2 | 2.17                     | 0.43              |
| 36:DN:17:ASP:CG   | 36:DN:17:ASP:O    | 2.55                     | 0.43              |
| 37:DO:85:VAL:HG21 | 37:DO:98:VAL:HG23 | 2.00                     | 0.43              |
| 27:DA:2393:A:O3'  | 38:DP:63:PRO:HD2  | 2.18                     | 0.43              |
| 40:DR:83:ILE:C    | 40:DR:85:PRO:HD2  | 2.38                     | 0.43              |
| 40:DR:92:GLY:N    | 40:DR:94:TYR:CE1  | 2.86                     | 0.43              |
| 42:DT:27:THR:HA   | 42:DT:87:ASP:HB2  | 2.00                     | 0.43              |
| 42:DT:96:ARG:HB3  | 42:DT:96:ARG:CZ   | 2.48                     | 0.43              |
| 45:DW:41:LYS:O    | 45:DW:42:ARG:C    | 2.56                     | 0.43              |
| 47:DY:80:GLY:O    | 47:DY:81:LYS:O    | 2.37                     | 0.43              |
| 1:AA:1049:U:O2'   | 1:AA:1050:G:P     | 2.76                     | 0.43              |
| 1:AA:1053:G:O2'   | 1:AA:1054:C:P     | 2.77                     | 0.43              |
| 1:AA:106:C:H2'    | 1:AA:107:G:C8     | 2.53                     | 0.43              |
| 1:AA:1102:A:H2'   | 1:AA:1103:C:C6    | 2.54                     | 0.43              |
| 1:AA:1296:C:H4'   | 1:AA:1302:U:C5    | 2.54                     | 0.43              |
| 1:AA:1296:C:H5''  | 1:AA:1297:C:OP2   | 2.19                     | 0.43              |
| 1:AA:1494:G:N7    | 26:AZ:1:KBE:HAA   | 2.33                     | 0.43              |
| 1:AA:16:A:N1      | 1:AA:920:U:C2     | 2.86                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:20:U:H2'     | 1:AA:21:G:H5'     | 2.00                     | 0.43              |
| 1:AA:268:C:C5     | 1:AA:269:C:H5     | 2.37                     | 0.43              |
| 1:AA:457:C:H2'    | 1:AA:458:C:C6     | 2.52                     | 0.43              |
| 1:AA:61:G:H2'     | 1:AA:62:U:C6      | 2.53                     | 0.43              |
| 2:AB:19:HIS:CG    | 2:AB:20:GLU:H     | 2.37                     | 0.43              |
| 3:AC:183:ASP:O    | 3:AC:201:TYR:HA   | 2.19                     | 0.43              |
| 3:AC:24:ALA:HB3   | 3:AC:29:TYR:CD1   | 2.53                     | 0.43              |
| 3:AC:55:VAL:HG12  | 3:AC:55:VAL:O     | 2.18                     | 0.43              |
| 4:AD:153:ARG:HH21 | 4:AD:181:MET:HB2  | 1.83                     | 0.43              |
| 4:AD:204:ILE:H    | 4:AD:204:ILE:HG12 | 1.71                     | 0.43              |
| 4:AD:28:SER:HB2   | 4:AD:30:LYS:CG    | 2.48                     | 0.43              |
| 5:AE:33:VAL:HG23  | 5:AE:43:LEU:CD1   | 2.26                     | 0.43              |
| 6:AF:77:ARG:O     | 6:AF:80:ARG:N     | 2.51                     | 0.43              |
| 8:AH:100:ILE:CD1  | 8:AH:124:ALA:HB3  | 2.48                     | 0.43              |
| 5:AE:148:VAL:CG2  | 8:AH:107:LEU:HD13 | 2.48                     | 0.43              |
| 8:AH:23:SER:HA    | 8:AH:63:LEU:HD22  | 2.00                     | 0.43              |
| 9:AI:95:LYS:HD3   | 9:AI:96:LEU:N     | 2.33                     | 0.43              |
| 17:AQ:19:VAL:O    | 17:AQ:43:LEU:HA   | 2.18                     | 0.43              |
| 17:AQ:81:ARG:C    | 17:AQ:83:ASP:H    | 2.21                     | 0.43              |
| 20:AT:86:ARG:HH11 | 20:AT:86:ARG:HG3  | 1.83                     | 0.43              |
| 23:AW:24:C:H2'    | 23:AW:25:A:H5'    | 2.01                     | 0.43              |
| 24:AX:8:U:H5'     | 24:AX:48:C:O2'    | 2.18                     | 0.43              |
| 39:BQ:80:GLU:HB2  | 49:B0:5:LYS:HE3   | 2.00                     | 0.43              |
| 50:B1:51:VAL:O    | 50:B1:52:ARG:C    | 2.57                     | 0.43              |
| 52:B3:24:LYS:O    | 52:B3:27:GLY:HA2  | 2.18                     | 0.43              |
| 55:B6:28:ARG:HG2  | 55:B6:28:ARG:HH11 | 1.83                     | 0.43              |
| 57:B8:10:ALA:C    | 57:B8:12:LYS:N    | 2.71                     | 0.43              |
| 58:B9:26:ILE:HG22 | 58:B9:27:CYS:N    | 2.33                     | 0.43              |
| 27:BA:1204:A:C2   | 27:BA:1241:A:N1   | 2.87                     | 0.43              |
| 27:BA:1281:G:H5'  | 27:BA:1282:U:OP2  | 2.19                     | 0.43              |
| 27:BA:1813:G:H2'  | 27:BA:1814:G:H5'  | 1.99                     | 0.43              |
| 27:BA:1855:G:O2'  | 27:BA:1856:G:H5'  | 2.19                     | 0.43              |
| 27:BA:1936:A:H4'  | 27:BA:1937:A:H5'  | 2.01                     | 0.43              |
| 27:BA:1956:U:O2'  | 27:BA:1957:C:H5'  | 2.17                     | 0.43              |
| 27:BA:2115:G:C2   | 27:BA:2117:A:N7   | 2.86                     | 0.43              |
| 27:BA:2182:G:H2'  | 27:BA:2183:C:C6   | 2.53                     | 0.43              |
| 27:BA:2199:A:N1   | 27:BA:2226:C:N4   | 2.55                     | 0.43              |
| 27:BA:2093:G:O6   | 27:BA:2225:A:C8   | 2.72                     | 0.43              |
| 27:BA:2283:C:C2   | 27:BA:2389:G:C2   | 3.07                     | 0.43              |
| 27:BA:2439:A:H4'  | 27:BA:2440:C:H3'  | 2.00                     | 0.43              |
| 27:BA:2732:G:C3'  | 27:BA:2733:A:C5'  | 2.88                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:2811:G:OP1   | 31:BE:60:ASN:HB2  | 2.18                     | 0.43              |
| 27:BA:321:G:O2'    | 27:BA:322:A:OP1   | 2.26                     | 0.43              |
| 27:BA:447:A:C8     | 27:BA:473:G:C6    | 3.07                     | 0.43              |
| 27:BA:580:C:H2'    | 27:BA:581:C:C6    | 2.54                     | 0.43              |
| 27:BA:770:G:C6     | 27:BA:771:G:N7    | 2.87                     | 0.43              |
| 27:BA:775:G:O2'    | 27:BA:794:G:N7    | 2.43                     | 0.43              |
| 28:BB:66:A:O2'     | 28:BB:67:G:OP2    | 2.31                     | 0.43              |
| 28:BB:69:G:O2'     | 28:BB:70:C:H5'    | 2.18                     | 0.43              |
| 31:BE:51:PHE:C     | 31:BE:74:PRO:HB2  | 2.39                     | 0.43              |
| 33:BG:102:PHE:O    | 33:BG:105:LYS:HG3 | 2.19                     | 0.43              |
| 33:BG:125:PHE:O    | 33:BG:126:ASP:O   | 2.35                     | 0.43              |
| 33:BG:166:ASP:O    | 33:BG:170:ARG:N   | 2.43                     | 0.43              |
| 35:BI:123:LEU:HD11 | 35:BI:144:VAL:CG1 | 2.48                     | 0.43              |
| 36:BN:95:PRO:O     | 36:BN:96:GLU:C    | 2.57                     | 0.43              |
| 38:BP:139:LYS:O    | 38:BP:141:ALA:N   | 2.42                     | 0.43              |
| 38:BP:38:GLN:CG    | 38:BP:39:LYS:H    | 2.29                     | 0.43              |
| 40:BR:55:ALA:CB    | 40:BR:79:LEU:HD22 | 2.48                     | 0.43              |
| 40:BR:67:LEU:HD22  | 40:BR:76:VAL:CG2  | 2.46                     | 0.43              |
| 40:BR:73:VAL:O     | 40:BR:76:VAL:HB   | 2.19                     | 0.43              |
| 42:BT:109:GLU:O    | 42:BT:112:ARG:N   | 2.51                     | 0.43              |
| 31:BE:14:ILE:HD12  | 42:BT:14:TYR:CZ   | 2.53                     | 0.43              |
| 48:BZ:8:TYR:HE2    | 48:BZ:34:ARG:CD   | 2.30                     | 0.43              |
| 48:BZ:68:THR:CA    | 48:BZ:90:LEU:HD12 | 2.46                     | 0.43              |
| 1:CA:1050:G:N2     | 1:CA:1209:C:H1'   | 2.33                     | 0.43              |
| 1:CA:1175:G:C2     | 1:CA:1176:A:C5    | 3.06                     | 0.43              |
| 1:CA:179:A:C4      | 1:CA:180:U:H5     | 2.35                     | 0.43              |
| 1:CA:17:U:H2'      | 1:CA:18:C:H6      | 1.75                     | 0.43              |
| 1:CA:200:G:H2'     | 1:CA:201:C:H6     | 1.81                     | 0.43              |
| 1:CA:260:G:C4      | 1:CA:261:U:C5     | 3.07                     | 0.43              |
| 1:CA:355:C:C4      | 1:CA:356:A:C5     | 3.07                     | 0.43              |
| 1:CA:367:U:OP1     | 1:CA:395:C:H1'    | 2.18                     | 0.43              |
| 1:CA:838:G:O2'     | 1:CA:839:U:H5''   | 2.19                     | 0.43              |
| 1:CA:857:C:H2'     | 1:CA:858:G:O4'    | 2.19                     | 0.43              |
| 1:CA:947:G:H4'     | 13:CM:109:THR:HG1 | 1.83                     | 0.43              |
| 1:CA:961:U:O2'     | 1:CA:962:C:O5'    | 2.37                     | 0.43              |
| 2:CB:105:PHE:C     | 2:CB:107:THR:N    | 2.71                     | 0.43              |
| 2:CB:7:VAL:O       | 2:CB:11:LEU:HG    | 2.19                     | 0.43              |
| 3:CC:192:THR:CG2   | 3:CC:192:THR:O    | 2.65                     | 0.43              |
| 3:CC:27:LYS:HZ3    | 3:CC:27:LYS:HB3   | 1.83                     | 0.43              |
| 3:CC:6:HIS:HD2     | 3:CC:8:ILE:H      | 1.65                     | 0.43              |
| 4:CD:11:LEU:O      | 4:CD:13:ARG:N     | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:CF:3:ARG:HG2    | 6:CF:93:SER:OG    | 2.18                     | 0.43              |
| 7:CG:120:ILE:HG22 | 7:CG:124:LEU:CD1  | 2.46                     | 0.43              |
| 7:CG:149:ARG:O    | 7:CG:150:ALA:C    | 2.57                     | 0.43              |
| 13:CM:6:GLY:C     | 13:CM:7:VAL:HG23  | 2.39                     | 0.43              |
| 16:CP:15:PRO:O    | 16:CP:16:HIS:ND1  | 2.52                     | 0.43              |
| 16:CP:75:ARG:O    | 16:CP:77:ALA:N    | 2.51                     | 0.43              |
| 16:CP:9:PHE:HE2   | 16:CP:18:ARG:HB3  | 1.83                     | 0.43              |
| 6:CF:100:ASN:HD22 | 18:CR:23:LYS:HE3  | 1.82                     | 0.43              |
| 20:CT:34:LYS:O    | 20:CT:37:SER:HB2  | 2.19                     | 0.43              |
| 20:CT:74:LYS:HB3  | 20:CT:75:ASN:H    | 1.50                     | 0.43              |
| 25:CY:25:A:H2'    | 25:CY:26:C:H5'    | 2.00                     | 0.43              |
| 50:D1:70:VAL:O    | 50:D1:73:LEU:HB2  | 2.19                     | 0.43              |
| 54:D5:25:LEU:HD23 | 54:D5:26:THR:H    | 1.83                     | 0.43              |
| 54:D5:31:VAL:CG2  | 54:D5:40:LYS:HE2  | 2.48                     | 0.43              |
| 57:D8:52:LYS:H    | 57:D8:53:PRO:HD2  | 1.78                     | 0.43              |
| 27:DA:1157:G:O2'  | 27:DA:1158:C:C5'  | 2.67                     | 0.43              |
| 27:DA:1191:G:C2   | 27:DA:1192:G:C8   | 3.06                     | 0.43              |
| 27:DA:1192:G:O2'  | 27:DA:1193:G:H5'  | 2.19                     | 0.43              |
| 27:DA:1304:C:C4   | 27:DA:1305:C:C5   | 3.07                     | 0.43              |
| 27:DA:1385:G:C4'  | 27:DA:1386:C:OP1  | 2.63                     | 0.43              |
| 27:DA:1479:G:H5'  | 27:DA:1558:A:C2   | 2.52                     | 0.43              |
| 27:DA:1833:U:C4   | 27:DA:1834:U:C4   | 3.07                     | 0.43              |
| 27:DA:195:A:H61   | 27:DA:198:C:H3'   | 1.84                     | 0.43              |
| 27:DA:2016:U:O2'  | 27:DA:2017:U:H5'  | 2.18                     | 0.43              |
| 27:DA:2070:G:C4   | 27:DA:2071:A:C8   | 3.06                     | 0.43              |
| 27:DA:2125:G:H21  | 27:DA:2174:C:N4   | 2.14                     | 0.43              |
| 27:DA:2141:G:H2'  | 27:DA:2142:C:O4'  | 2.18                     | 0.43              |
| 27:DA:2134:A:C8   | 27:DA:2158:A:C2   | 3.06                     | 0.43              |
| 27:DA:2159:G:C3'  | 27:DA:2160:G:H5'' | 2.48                     | 0.43              |
| 27:DA:2287:A:O2'  | 27:DA:2288:A:O5'  | 2.36                     | 0.43              |
| 27:DA:2382:G:O2'  | 27:DA:2383:G:P    | 2.77                     | 0.43              |
| 27:DA:2721:A:C2   | 27:DA:2873:A:C4   | 3.06                     | 0.43              |
| 27:DA:2756:U:H1'  | 27:DA:2757:A:C5'  | 2.40                     | 0.43              |
| 27:DA:353:G:N2    | 27:DA:354:G:C4    | 2.86                     | 0.43              |
| 27:DA:524:U:C2    | 27:DA:525:U:C5    | 3.06                     | 0.43              |
| 27:DA:534:U:O2'   | 27:DA:535:C:H5'   | 2.18                     | 0.43              |
| 27:DA:565:C:O2'   | 27:DA:566:U:H5'   | 2.18                     | 0.43              |
| 27:DA:815:C:C2    | 27:DA:816:C:C5    | 3.07                     | 0.43              |
| 27:DA:95:G:H4'    | 51:D2:46:GLN:OE1  | 2.18                     | 0.43              |
| 27:DA:971:C:H2'   | 27:DA:972:G:O4'   | 2.19                     | 0.43              |
| 28:DB:16:G:C6     | 28:DB:17:C:C4     | 3.07                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DC:56:GLN:NE2  | 29:DC:173:ALA:CB   | 2.82                     | 0.43              |
| 30:DD:139:GLY:O   | 30:DD:164:GLN:HG3  | 2.19                     | 0.43              |
| 32:DF:32:LEU:HD22 | 32:DF:112:MET:HE3  | 1.99                     | 0.43              |
| 32:DF:46:ARG:HB3  | 32:DF:48:THR:HG23  | 1.99                     | 0.43              |
| 33:DG:18:GLU:HB3  | 33:DG:175:LEU:CD2  | 2.48                     | 0.43              |
| 35:DI:128:LEU:O   | 35:DI:137:PRO:HA   | 2.19                     | 0.43              |
| 35:DI:25:TYR:CE2  | 35:DI:29:TYR:CD2   | 3.06                     | 0.43              |
| 35:DI:39:ALA:O    | 35:DI:44:LEU:HD22  | 2.19                     | 0.43              |
| 35:DI:82:ARG:HH11 | 35:DI:82:ARG:HG3   | 1.84                     | 0.43              |
| 35:DI:88:ILE:CG2  | 35:DI:90:GLY:O     | 2.66                     | 0.43              |
| 38:DP:114:ILE:O   | 38:DP:130:PHE:HA   | 2.17                     | 0.43              |
| 39:DQ:126:PRO:O   | 39:DQ:127:ILE:HG23 | 2.17                     | 0.43              |
| 40:DR:88:ARG:HD2  | 40:DR:89:ASP:CG    | 2.39                     | 0.43              |
| 42:DT:35:LYS:C    | 42:DT:37:GLY:H     | 2.22                     | 0.43              |
| 1:AA:1051:C:H6    | 1:AA:1051:C:O5'    | 2.01                     | 0.43              |
| 1:AA:1096:C:O2'   | 1:AA:1097:C:H5'    | 2.18                     | 0.43              |
| 1:AA:1106:G:H2'   | 1:AA:1107:C:H6     | 1.83                     | 0.43              |
| 1:AA:1305:G:OP2   | 21:AU:2:GLY:N      | 2.51                     | 0.43              |
| 1:AA:1434:A:H2'   | 1:AA:1435:G:H5'    | 2.00                     | 0.43              |
| 1:AA:345:C:H5'    | 42:BT:36:GLU:HG3   | 2.00                     | 0.43              |
| 1:AA:674:G:C6     | 1:AA:675:A:N6      | 2.87                     | 0.43              |
| 2:AB:71:VAL:HA    | 2:AB:93:VAL:HG23   | 2.00                     | 0.43              |
| 3:AC:12:LEU:HD12  | 3:AC:18:TRP:CZ2    | 2.53                     | 0.43              |
| 3:AC:89:GLU:HG3   | 3:AC:90:GLU:OE1    | 2.19                     | 0.43              |
| 5:AE:101:ILE:HG12 | 5:AE:119:LEU:HD23  | 2.00                     | 0.43              |
| 7:AG:23:VAL:O     | 7:AG:26:PHE:N      | 2.51                     | 0.43              |
| 9:AI:10:ARG:HD3   | 9:AI:75:ASP:HB3    | 2.00                     | 0.43              |
| 1:AA:1343:G:H1'   | 9:AI:121:ARG:NH1   | 2.33                     | 0.43              |
| 9:AI:5:TYR:CG     | 9:AI:6:GLY:N       | 2.86                     | 0.43              |
| 1:AA:973:G:H4'    | 10:AJ:54:PHE:O     | 2.19                     | 0.43              |
| 13:AM:114:ARG:HG2 | 13:AM:114:ARG:HH11 | 1.83                     | 0.43              |
| 13:AM:80:ARG:O    | 13:AM:83:ASP:N     | 2.48                     | 0.43              |
| 15:AO:30:ALA:HA   | 15:AO:33:THR:HB    | 2.00                     | 0.43              |
| 15:AO:44:LYS:HB2  | 15:AO:44:LYS:HE3   | 1.79                     | 0.43              |
| 17:AQ:9:VAL:HA    | 17:AQ:55:ASP:O     | 2.18                     | 0.43              |
| 17:AQ:86:GLU:OE1  | 17:AQ:86:GLU:HA    | 2.19                     | 0.43              |
| 18:AR:53:ARG:CZ   | 18:AR:60:ALA:N     | 2.80                     | 0.43              |
| 6:AF:91:VAL:HG13  | 18:AR:72:ARG:CZ    | 2.48                     | 0.43              |
| 25:AY:14:A:C8     | 25:AY:21:A:N6      | 2.87                     | 0.43              |
| 25:AY:48:C:N4     | 25:AY:64:G:H1      | 2.17                     | 0.43              |
| 50:B1:3:LYS:HG3   | 50:B1:4:VAL:HG12   | 2.00                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:B2:42:GLY:C     | 51:B2:44:LEU:H    | 2.20                     | 0.43              |
| 51:B2:3:LEU:O      | 51:B2:6:VAL:HG23  | 2.19                     | 0.43              |
| 27:BA:105:C:O2'    | 47:BY:2:ARG:CB    | 2.65                     | 0.43              |
| 27:BA:1477:A:C4    | 27:BA:1515:G:N2   | 2.87                     | 0.43              |
| 27:BA:1300:U:H1'   | 27:BA:1626:G:C2   | 2.54                     | 0.43              |
| 27:BA:1658:C:O2    | 27:BA:2003:G:C2   | 2.72                     | 0.43              |
| 27:BA:1741:A:O2'   | 27:BA:1742:G:O4'  | 2.37                     | 0.43              |
| 27:BA:1999:C:O2'   | 27:BA:2000:G:H5'  | 2.18                     | 0.43              |
| 27:BA:2048:G:C6    | 27:BA:2621:A:C2   | 3.06                     | 0.43              |
| 27:BA:2405:G:O2'   | 27:BA:2411:A:N6   | 2.51                     | 0.43              |
| 27:BA:2525:G:N1    | 27:BA:2526:G:C5   | 2.86                     | 0.43              |
| 27:BA:2619:C:OP1   | 31:BE:152:LYS:HE3 | 2.18                     | 0.43              |
| 27:BA:271(R):G:H2' | 27:BA:271(S):G:H8 | 1.83                     | 0.43              |
| 27:BA:2731:G:O5'   | 27:BA:2731:G:C8   | 2.69                     | 0.43              |
| 27:BA:2748:A:C8    | 27:BA:2754:U:O4   | 2.72                     | 0.43              |
| 27:BA:287:C:C2     | 27:BA:288:C:C6    | 3.07                     | 0.43              |
| 27:BA:287:C:H2'    | 27:BA:288:C:H6    | 1.83                     | 0.43              |
| 27:BA:563:G:C2     | 27:BA:564:C:C4    | 3.07                     | 0.43              |
| 27:BA:769:G:O2'    | 27:BA:770:G:H5'   | 2.18                     | 0.43              |
| 30:BD:117:VAL:HG13 | 30:BD:118:VAL:N   | 2.33                     | 0.43              |
| 30:BD:14:ARG:HG3   | 30:BD:15:PHE:CE1  | 2.54                     | 0.43              |
| 30:BD:24:ILE:CG1   | 30:BD:25:THR:H    | 2.24                     | 0.43              |
| 32:BF:11:VAL:CG1   | 32:BF:12:LEU:N    | 2.79                     | 0.43              |
| 34:BH:71:LEU:H     | 34:BH:74:ASN:ND2  | 2.15                     | 0.43              |
| 35:BI:130:TYR:O    | 35:BI:131:LYS:O   | 2.35                     | 0.43              |
| 36:BN:118:LYS:O    | 36:BN:121:LYS:HE3 | 2.18                     | 0.43              |
| 38:BP:58:THR:O     | 38:BP:61:ARG:CZ   | 2.66                     | 0.43              |
| 39:BQ:55:VAL:O     | 39:BQ:59:ARG:HA   | 2.18                     | 0.43              |
| 40:BR:13:HIS:O     | 40:BR:16:HIS:N    | 2.43                     | 0.43              |
| 40:BR:48:VAL:O     | 40:BR:50:HIS:N    | 2.51                     | 0.43              |
| 41:BS:33:LYS:O     | 41:BS:34:HIS:CD2  | 2.72                     | 0.43              |
| 41:BS:93:LYS:O     | 41:BS:93:LYS:HG3  | 2.18                     | 0.43              |
| 42:BT:35:LYS:O     | 42:BT:37:GLY:N    | 2.52                     | 0.43              |
| 42:BT:65:LYS:HA    | 42:BT:65:LYS:HZ3  | 1.83                     | 0.43              |
| 43:BU:85:LYS:HD3   | 43:BU:117:GLN:NE2 | 2.32                     | 0.43              |
| 44:BV:82:ARG:CG    | 44:BV:82:ARG:HH11 | 2.31                     | 0.43              |
| 45:BW:2:GLU:HA     | 45:BW:107:LEU:O   | 2.19                     | 0.43              |
| 46:BX:31:HIS:CD2   | 46:BX:32:PRO:CD   | 3.01                     | 0.43              |
| 27:BA:71:A:C2      | 46:BX:31:HIS:CE1  | 2.94                     | 0.43              |
| 48:BZ:150:HIS:HB2  | 48:BZ:168:GLU:C   | 2.39                     | 0.43              |
| 1:CA:125:U:H2'     | 1:CA:126:G:C8     | 2.52                     | 0.43              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:CA:1428:A:C6      | 1:CA:1429:C:N4    | 2.87                     | 0.43              |
| 1:CA:1465:C:O2'     | 1:CA:1466:C:H5'   | 2.19                     | 0.43              |
| 1:CA:16:A:C2        | 1:CA:920:U:C2     | 3.06                     | 0.43              |
| 1:CA:228:A:H2'      | 1:CA:229:U:C6     | 2.52                     | 0.43              |
| 1:CA:256:U:C2       | 1:CA:257:G:C8     | 3.06                     | 0.43              |
| 1:CA:338:A:O2'      | 1:CA:339:C:H5'    | 2.19                     | 0.43              |
| 1:CA:390:C:H4'      | 16:CP:28:ARG:NH2  | 2.33                     | 0.43              |
| 1:CA:422:C:H5'      | 1:CA:423:G:OP1    | 2.18                     | 0.43              |
| 1:CA:693:G:O2'      | 1:CA:694:A:H5'    | 2.18                     | 0.43              |
| 1:CA:737:A:O2'      | 6:CF:72:VAL:CG1   | 2.64                     | 0.43              |
| 1:CA:787:A:O2'      | 1:CA:788:U:H5'    | 2.19                     | 0.43              |
| 1:CA:784:C:C4       | 1:CA:799:G:N1     | 2.87                     | 0.43              |
| 2:CB:19:HIS:CE1     | 2:CB:205:ASP:OD1  | 2.71                     | 0.43              |
| 4:CD:207:TYR:HD2    | 4:CD:207:TYR:HA   | 1.61                     | 0.43              |
| 4:CD:98:GLU:HG2     | 4:CD:189:PRO:HG2  | 2.00                     | 0.43              |
| 5:CE:105:VAL:O      | 5:CE:108:ALA:CB   | 2.62                     | 0.43              |
| 5:CE:139:LEU:HD22   | 5:CE:142:LEU:HD11 | 2.00                     | 0.43              |
| 7:CG:143:ARG:CB     | 7:CG:143:ARG:NH1  | 2.81                     | 0.43              |
| 8:CH:38:ILE:O       | 8:CH:41:ARG:HG2   | 2.18                     | 0.43              |
| 8:CH:48:TYR:O       | 8:CH:49:GLU:CB    | 2.67                     | 0.43              |
| 8:CH:6:ILE:HD11     | 8:CH:31:PHE:CD2   | 2.53                     | 0.43              |
| 11:CK:116:HIS:O     | 11:CK:117:ASN:HB2 | 2.19                     | 0.43              |
| 13:CM:45:VAL:C      | 13:CM:47:ASP:H    | 2.21                     | 0.43              |
| 13:CM:86:CYS:HA     | 19:CS:73:GLU:O    | 2.18                     | 0.43              |
| 17:CQ:25:ARG:HB3    | 17:CQ:38:ARG:O    | 2.19                     | 0.43              |
| 18:CR:66:LEU:O      | 18:CR:70:ILE:N    | 2.51                     | 0.43              |
| 20:CT:42:GLN:HG3    | 20:CT:43:LEU:HD23 | 2.01                     | 0.43              |
| 20:CT:57:ARG:HH11   | 20:CT:57:ARG:HB2  | 1.83                     | 0.43              |
| 1:CA:1400:C:O4'     | 22:CV:6:G:C6      | 2.72                     | 0.43              |
| 25:CY:25:A:O2'      | 25:CY:26:C:H5'    | 2.18                     | 0.43              |
| 27:DA:2261:C:OP2    | 49:D0:17:GLN:HG2  | 2.19                     | 0.43              |
| 27:DA:921:G:N2      | 49:D0:26:TYR:CD1  | 2.86                     | 0.43              |
| 49:D0:43:THR:O      | 49:D0:43:THR:HG23 | 2.19                     | 0.43              |
| 52:D3:50:VAL:HB     | 52:D3:53:LEU:HD12 | 2.00                     | 0.43              |
| 58:D9:29:ASN:HB2    | 58:D9:30:PRO:HD2  | 2.00                     | 0.43              |
| 27:DA:1028:A:H2'    | 27:DA:1029:A:C8   | 2.54                     | 0.43              |
| 27:DA:1190:G:H2'    | 27:DA:1191:G:H8   | 1.84                     | 0.43              |
| 27:DA:1332:G:C5'    | 27:DA:1333:C:OP2  | 2.63                     | 0.43              |
| 27:DA:1405:U:H2'    | 27:DA:1406:U:C6   | 2.53                     | 0.43              |
| 27:DA:1450(A):C:H2' | 27:DA:1451:C:C6   | 2.54                     | 0.43              |
| 27:DA:1525:G:O2'    | 27:DA:1526:G:H5'  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:154:G:H2'   | 27:DA:154(A):C:O2  | 2.18                     | 0.43              |
| 27:DA:1695:G:O2'  | 27:DA:1696:G:P     | 2.77                     | 0.43              |
| 27:DA:1835:G:C5'  | 27:DA:1836:C:OP2   | 2.66                     | 0.43              |
| 27:DA:1883:G:O2'  | 27:DA:1884:A:H8    | 2.01                     | 0.43              |
| 27:DA:1895:C:H2'  | 27:DA:1896:G:O4'   | 2.18                     | 0.43              |
| 27:DA:1906:G:N2   | 27:DA:1925:C:O2    | 2.51                     | 0.43              |
| 27:DA:2027:G:C4   | 27:DA:2028:U:C6    | 3.07                     | 0.43              |
| 27:DA:2036:C:C6   | 27:DA:2036:C:H5'   | 2.54                     | 0.43              |
| 27:DA:2228:G:P    | 30:DD:263:ARG:HH12 | 2.41                     | 0.43              |
| 27:DA:2466:C:H2'  | 27:DA:2467:C:C5'   | 2.47                     | 0.43              |
| 27:DA:2007:C:H5'  | 27:DA:2824:C:O4'   | 2.18                     | 0.43              |
| 27:DA:332:A:H4'   | 27:DA:333:G:OP1    | 2.17                     | 0.43              |
| 27:DA:374:A:H3'   | 27:DA:375:C:H6     | 1.82                     | 0.43              |
| 27:DA:622:G:O2'   | 27:DA:623:G:H5'    | 2.19                     | 0.43              |
| 27:DA:776:G:H1'   | 27:DA:793:A:C2     | 2.54                     | 0.43              |
| 27:DA:966:G:C6    | 27:DA:967:C:N4     | 2.86                     | 0.43              |
| 27:DA:972:G:N1    | 27:DA:973:A:N6     | 2.67                     | 0.43              |
| 27:DA:97:C:C5'    | 51:D2:2:LYS:HB2    | 2.48                     | 0.43              |
| 28:DB:103:G:C2'   | 28:DB:104:U:H5'    | 2.49                     | 0.43              |
| 29:DC:56:GLN:NE2  | 29:DC:173:ALA:HB1  | 2.34                     | 0.43              |
| 29:DC:99:ILE:HA   | 29:DC:103:ILE:CB   | 2.49                     | 0.43              |
| 30:DD:143:HIS:HA  | 30:DD:156:ALA:HB3  | 2.00                     | 0.43              |
| 33:DG:125:PHE:CZ  | 33:DG:170:ARG:HA   | 2.53                     | 0.43              |
| 33:DG:36:LYS:O    | 33:DG:160:VAL:HG23 | 2.19                     | 0.43              |
| 34:DH:102:ALA:CB  | 34:DH:116:GLU:HA   | 2.49                     | 0.43              |
| 38:DP:11:GLY:O    | 38:DP:12:ALA:C     | 2.55                     | 0.43              |
| 38:DP:146:VAL:CG1 | 38:DP:147:LEU:H    | 2.26                     | 0.43              |
| 38:DP:6:LEU:H     | 38:DP:6:LEU:HD23   | 1.83                     | 0.43              |
| 27:DA:1286:A:P    | 40:DR:105:ARG:HH11 | 2.42                     | 0.43              |
| 40:DR:48:VAL:HA   | 40:DR:51:LEU:HD11  | 2.00                     | 0.43              |
| 42:DT:1:MET:C     | 42:DT:3:ARG:N      | 2.71                     | 0.43              |
| 42:DT:92:GLY:O    | 42:DT:94:ALA:N     | 2.43                     | 0.43              |
| 48:DZ:27:MET:HE1  | 48:DZ:32:LEU:HD11  | 1.99                     | 0.43              |
| 48:DZ:62:ASP:C    | 48:DZ:64:GLN:H     | 2.22                     | 0.43              |
| 1:AA:1097:C:O2    | 1:AA:1169:A:H2     | 2.01                     | 0.43              |
| 1:AA:1248:A:C2'   | 1:AA:1249:C:C5'    | 2.97                     | 0.43              |
| 1:AA:1285:A:C5'   | 1:AA:1286:A:C8     | 2.99                     | 0.43              |
| 1:AA:159:G:H21    | 1:AA:161:A:H3'     | 1.84                     | 0.43              |
| 1:AA:189(B):C:N4  | 1:AA:189(I):G:H1   | 2.17                     | 0.43              |
| 1:AA:297:G:C5     | 1:AA:299:G:OP2     | 2.72                     | 0.43              |
| 1:AA:321:A:N7     | 1:AA:328:C:O2'     | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:705:U:H5     | 1:AA:706:A:C5     | 2.36                     | 0.43              |
| 1:AA:976:G:OP1    | 14:AN:32:SER:N    | 2.51                     | 0.43              |
| 1:AA:1158:C:O3'   | 2:AB:133:LYS:NZ   | 2.52                     | 0.43              |
| 2:AB:161:ALA:HA   | 2:AB:182:ILE:HG22 | 2.01                     | 0.43              |
| 2:AB:97:TRP:CZ2   | 2:AB:173:ALA:HA   | 2.54                     | 0.43              |
| 1:AA:1073:U:OP2   | 5:AE:57:LYS:HE3   | 2.18                     | 0.43              |
| 8:AH:17:THR:C     | 8:AH:20:TYR:H     | 2.20                     | 0.43              |
| 10:AJ:78:ASN:O    | 10:AJ:82:ILE:HG12 | 2.18                     | 0.43              |
| 15:AO:62:GLN:NE2  | 15:AO:66:LEU:CD1  | 2.82                     | 0.43              |
| 17:AQ:67:LYS:O    | 17:AQ:68:ARG:HB3  | 2.19                     | 0.43              |
| 18:AR:32:ARG:HH11 | 18:AR:65:ILE:HD13 | 1.84                     | 0.43              |
| 1:AA:1286:A:H2    | 21:AU:22:ARG:HH21 | 1.65                     | 0.43              |
| 24:AX:43:A:C2     | 24:AX:44:A:C2     | 3.06                     | 0.43              |
| 26:AZ:5:UAL:C     | 26:AZ:6:5OH:HS    | 2.49                     | 0.43              |
| 50:B1:52:ARG:CG   | 50:B1:53:VAL:N    | 2.81                     | 0.43              |
| 51:B2:28:LYS:CB   | 51:B2:57:ILE:HD12 | 2.48                     | 0.43              |
| 51:B2:9:GLN:OE1   | 51:B2:56:GLN:HG2  | 2.19                     | 0.43              |
| 54:B5:33:CYS:O    | 54:B5:34:PRO:C    | 2.57                     | 0.43              |
| 27:BA:1015:G:H5'' | 27:BA:1015:G:C8   | 2.51                     | 0.43              |
| 27:BA:1109:C:H5   | 27:BA:1110:G:C5   | 2.36                     | 0.43              |
| 27:BA:1231:G:H2'  | 27:BA:1232:G:C8   | 2.54                     | 0.43              |
| 27:BA:564:C:O2    | 27:BA:1253:A:H2   | 2.01                     | 0.43              |
| 27:BA:1722:A:N1   | 27:BA:1740:G:C8   | 2.77                     | 0.43              |
| 27:BA:1750:G:N2   | 27:BA:1751:C:C2   | 2.87                     | 0.43              |
| 27:BA:1801:G:OP2  | 30:BD:154:LYS:HE2 | 2.18                     | 0.43              |
| 27:BA:2197:U:C4   | 27:BA:2224:G:C2   | 3.06                     | 0.43              |
| 27:BA:2294:C:OP1  | 41:BS:92:TYR:HE1  | 2.02                     | 0.43              |
| 27:BA:2393:A:C2'  | 27:BA:2394:C:H5'  | 2.48                     | 0.43              |
| 27:BA:2460:U:C2'  | 27:BA:2461:C:H5'  | 2.49                     | 0.43              |
| 27:BA:2467:C:H2'  | 27:BA:2468:G:O4'  | 2.18                     | 0.43              |
| 27:BA:252:G:H2'   | 27:BA:253:C:C6    | 2.52                     | 0.43              |
| 27:BA:2694:G:C2'  | 27:BA:2695:C:O5'  | 2.66                     | 0.43              |
| 27:BA:302:C:H2'   | 27:BA:303:U:H6    | 1.82                     | 0.43              |
| 27:BA:341:G:N1    | 27:BA:342:G:C5    | 2.87                     | 0.43              |
| 27:BA:224:G:N7    | 27:BA:420:C:H4'   | 2.34                     | 0.43              |
| 27:BA:538:G:H5'   | 36:BN:5:VAL:HG21  | 2.00                     | 0.43              |
| 27:BA:563:G:C6    | 27:BA:564:C:N4    | 2.87                     | 0.43              |
| 27:BA:587:C:O5'   | 27:BA:587:C:C6    | 2.57                     | 0.43              |
| 27:BA:819:A:H2    | 27:BA:943:U:O4'   | 2.02                     | 0.43              |
| 27:BA:92:A:O2'    | 27:BA:93:G:H8     | 2.01                     | 0.43              |
| 27:BA:951:C:N4    | 27:BA:952:G:O6    | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BB:43:C:C4      | 28:BB:45:A:N6      | 2.86                     | 0.43              |
| 29:BC:72:VAL:HG11  | 29:BC:161:ILE:HA   | 2.00                     | 0.43              |
| 30:BD:101:GLU:OE1  | 30:BD:103:ARG:CD   | 2.57                     | 0.43              |
| 31:BE:59:VAL:CG2   | 31:BE:60:ASN:N     | 2.52                     | 0.43              |
| 31:BE:57:LYS:C     | 31:BE:59:VAL:HG12  | 2.39                     | 0.43              |
| 32:BF:130:ALA:O    | 32:BF:132:VAL:N    | 2.52                     | 0.43              |
| 32:BF:7:TYR:HB3    | 32:BF:16:GLY:H     | 1.84                     | 0.43              |
| 33:BG:145:THR:OG1  | 33:BG:147:ASP:CG   | 2.57                     | 0.43              |
| 33:BG:26:GLN:O     | 33:BG:28:VAL:N     | 2.49                     | 0.43              |
| 35:BI:45:LYS:HA    | 35:BI:48:GLU:HG3   | 2.01                     | 0.43              |
| 36:BN:130:HIS:O    | 36:BN:132:ALA:N    | 2.51                     | 0.43              |
| 36:BN:30:ILE:HD13  | 36:BN:54:VAL:CG2   | 2.49                     | 0.43              |
| 37:BO:88:ASN:ND2   | 37:BO:90:GLN:OE1   | 2.51                     | 0.43              |
| 38:BP:47:ASP:CB    | 38:BP:48:PRO:CA    | 2.88                     | 0.43              |
| 38:BP:91:PHE:N     | 38:BP:91:PHE:CD1   | 2.86                     | 0.43              |
| 38:BP:97:PRO:C     | 38:BP:99:LEU:H     | 2.12                     | 0.43              |
| 39:BQ:31:ASP:N     | 39:BQ:106:VAL:O    | 2.49                     | 0.43              |
| 27:BA:910:A:C6     | 39:BQ:13:GLN:NE2   | 2.86                     | 0.43              |
| 40:BR:44:LEU:HD13  | 40:BR:44:LEU:C     | 2.38                     | 0.43              |
| 40:BR:76:VAL:HG13  | 40:BR:77:ARG:N     | 2.34                     | 0.43              |
| 46:BX:18:TYR:C     | 46:BX:20:GLY:N     | 2.72                     | 0.43              |
| 47:BY:11:ASP:O     | 47:BY:27:VAL:N     | 2.51                     | 0.43              |
| 47:BY:30:VAL:HG22  | 47:BY:37:VAL:HG12  | 2.00                     | 0.43              |
| 48:BZ:99:VAL:O     | 48:BZ:101:LEU:HD13 | 2.19                     | 0.43              |
| 48:BZ:127:VAL:HG22 | 48:BZ:128:SER:N    | 2.34                     | 0.43              |
| 48:BZ:75:LEU:HA    | 48:BZ:75:LEU:HD22  | 1.79                     | 0.43              |
| 1:CA:1097:C:H2'    | 1:CA:1097:C:O2     | 2.18                     | 0.43              |
| 1:CA:1288:A:C6     | 1:CA:1289:A:C5     | 3.07                     | 0.43              |
| 1:CA:1354:C:H2'    | 1:CA:1355:G:H8     | 1.83                     | 0.43              |
| 1:CA:328:C:C2'     | 1:CA:328:C:O2      | 2.66                     | 0.43              |
| 1:CA:397:A:C2'     | 1:CA:399:G:OP2     | 2.64                     | 0.43              |
| 1:CA:445:G:H1      | 1:CA:489:C:N4      | 2.13                     | 0.43              |
| 1:CA:453:A:C6      | 1:CA:454:C:C4      | 3.07                     | 0.43              |
| 1:CA:533:A:C6      | 1:CA:536:C:C4      | 3.07                     | 0.43              |
| 1:CA:629:G:N2      | 1:CA:630:G:N3      | 2.67                     | 0.43              |
| 1:CA:965:A:C5'     | 1:CA:966:G:OP1     | 2.66                     | 0.43              |
| 2:CB:97:TRP:O      | 2:CB:97:TRP:CE3    | 2.71                     | 0.43              |
| 5:CE:72:GLN:O      | 5:CE:73:ASN:HB3    | 2.18                     | 0.43              |
| 6:CF:5:GLU:O       | 6:CF:90:VAL:HA     | 2.19                     | 0.43              |
| 6:CF:80:ARG:H      | 6:CF:80:ARG:HG2    | 1.63                     | 0.43              |
| 1:CA:878:G:H1'     | 8:CH:3:THR:HG21    | 2.01                     | 0.43              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 13:CM:115:LYS:O  | 13:CM:117:VAL:HG23 | 2.18                     | 0.43              |
| 13:CM:14:ARG:HB2 | 13:CM:41:PRO:O     | 2.19                     | 0.43              |
| 13:CM:23:TYR:HE1 | 13:CM:71:ARG:CA    | 2.31                     | 0.43              |
| 13:CM:83:ASP:OD2 | 13:CM:83:ASP:N     | 2.50                     | 0.43              |
| 17:CQ:40:LYS:HD3 | 17:CQ:42:TYR:CE2   | 2.54                     | 0.43              |
| 19:CS:4:SER:O    | 19:CS:5:LEU:HB3    | 2.17                     | 0.43              |
| 23:CW:20:A:C2    | 23:CW:47:C:C2      | 3.06                     | 0.43              |
| 25:CY:71:A:H2'   | 25:CY:72:G:O4'     | 2.19                     | 0.43              |
| 49:D0:65:GLY:HA3 | 49:D0:81:VAL:HG12  | 2.01                     | 0.43              |
| 27:DA:1223:G:H5' | 27:DA:1224:C:OP2   | 2.18                     | 0.43              |
| 27:DA:1237:A:C2  | 27:DA:1238:G:N3    | 2.82                     | 0.43              |
| 27:DA:1623:G:O2' | 27:DA:1624:G:H5'   | 2.19                     | 0.43              |
| 27:DA:190:A:C4   | 27:DA:207:A:C2     | 3.07                     | 0.43              |
| 27:DA:195:A:C8   | 27:DA:197:A:OP1    | 2.71                     | 0.43              |
| 27:DA:1648:C:C2  | 27:DA:2010:G:N2    | 2.86                     | 0.43              |
| 27:DA:2428:G:H4' | 27:DA:2429:G:C8    | 2.53                     | 0.43              |
| 27:DA:2432:A:C5  | 27:DA:2433:A:C5    | 3.07                     | 0.43              |
| 27:DA:2469:A:N6  | 27:DA:2481:G:C1'   | 2.82                     | 0.43              |
| 27:DA:2693:A:H2' | 27:DA:2694:G:H8    | 1.84                     | 0.43              |
| 27:DA:280:C:N4   | 27:DA:361:G:C6     | 2.85                     | 0.43              |
| 27:DA:413:C:O2'  | 27:DA:1880:C:H1'   | 2.18                     | 0.43              |
| 27:DA:543:C:N3   | 27:DA:551:G:C2     | 2.86                     | 0.43              |
| 27:DA:626:U:H5'  | 27:DA:627:A:C5'    | 2.49                     | 0.43              |
| 27:DA:882:G:H2'  | 27:DA:883:G:C8     | 2.54                     | 0.43              |
| 27:DA:985:C:C6   | 27:DA:986:C:H5     | 2.36                     | 0.43              |
| 28:DB:12:C:H6    | 28:DB:12:C:OP2     | 2.01                     | 0.43              |
| 31:DE:9:VAL:CG2  | 31:DE:10:GLY:N     | 2.81                     | 0.43              |
| 31:DE:173:VAL:O  | 31:DE:174:ASP:O    | 2.37                     | 0.43              |
| 32:DF:141:ALA:O  | 32:DF:144:LYS:CB   | 2.61                     | 0.43              |
| 34:DH:86:GLU:HB2 | 34:DH:132:ARG:HH11 | 1.84                     | 0.43              |
| 35:DI:100:ALA:O  | 35:DI:101:LEU:HB2  | 2.18                     | 0.43              |
| 36:DN:97:ARG:HA  | 36:DN:100:GLU:HG3  | 2.01                     | 0.43              |
| 36:DN:19:GLU:HB2 | 36:DN:59:LYS:HB3   | 2.00                     | 0.43              |
| 39:DQ:29:PHE:HB3 | 39:DQ:30:GLY:H     | 1.43                     | 0.43              |
| 41:DS:40:ILE:O   | 41:DS:42:ASP:OD1   | 2.36                     | 0.43              |
| 46:DX:47:PHE:C   | 46:DX:48:LYS:HD2   | 2.38                     | 0.43              |
| 46:DX:5:TYR:HD1  | 46:DX:5:TYR:H      | 1.66                     | 0.43              |
| 47:DY:28:LYS:CA  | 47:DY:38:ILE:HB    | 2.48                     | 0.43              |
| 47:DY:6:HIS:CD2  | 47:DY:35:TYR:CE1   | 3.07                     | 0.43              |
| 47:DY:46:LYS:N   | 47:DY:62:GLU:CD    | 2.72                     | 0.43              |
| 48:DZ:94:PRO:CB  | 48:DZ:126:LYS:NZ   | 2.82                     | 0.43              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 48:DZ:78:ARG:H      | 48:DZ:78:ARG:HD2  | 1.82                     | 0.43              |
| 1:AA:1358:U:C5      | 1:AA:1359:C:C4    | 3.06                     | 0.43              |
| 1:AA:148:G:H2'      | 1:AA:149:A:H8     | 1.83                     | 0.43              |
| 1:AA:154:C:C2       | 1:AA:168:G:N2     | 2.87                     | 0.43              |
| 1:AA:219:C:H2'      | 1:AA:220:G:O4'    | 2.19                     | 0.43              |
| 1:AA:619:U:O2       | 4:AD:133:VAL:HA   | 2.18                     | 0.43              |
| 1:AA:768:A:N3       | 1:AA:1512:U:O2'   | 2.49                     | 0.43              |
| 1:AA:824:C:O2'      | 1:AA:825:G:H5'    | 2.19                     | 0.43              |
| 1:AA:905:U:C5       | 1:AA:906:G:C5     | 3.07                     | 0.43              |
| 2:AB:113:HIS:C      | 2:AB:115:LEU:H    | 2.22                     | 0.43              |
| 4:AD:173:TRP:HB3    | 4:AD:187:ARG:NH1  | 2.33                     | 0.43              |
| 5:AE:69:VAL:HA      | 5:AE:70:PRO:HD3   | 1.80                     | 0.43              |
| 7:AG:26:PHE:O       | 7:AG:30:ILE:HG12  | 2.18                     | 0.43              |
| 10:AJ:8:LEU:HD21    | 10:AJ:96:ILE:HG22 | 1.99                     | 0.43              |
| 12:AL:116:LYS:O     | 12:AL:117:TYR:CB  | 2.63                     | 0.43              |
| 14:AN:40:CYS:O      | 14:AN:42:ILE:N    | 2.52                     | 0.43              |
| 19:AS:32:LYS:HB2    | 19:AS:32:LYS:HE3  | 1.88                     | 0.43              |
| 19:AS:49:ILE:HG22   | 19:AS:50:ALA:N    | 2.34                     | 0.43              |
| 20:AT:32:ALA:O      | 20:AT:33:ILE:C    | 2.57                     | 0.43              |
| 24:AX:2:G:C4        | 24:AX:3:C:C5      | 3.07                     | 0.43              |
| 25:AY:63:C:H2'      | 25:AY:64:G:H8     | 1.78                     | 0.43              |
| 27:BA:372:G:H5'     | 50:B1:66:HIS:NE2  | 2.34                     | 0.43              |
| 51:B2:28:LYS:O      | 51:B2:29:LYS:C    | 2.57                     | 0.43              |
| 51:B2:45:SER:O      | 51:B2:46:GLN:NE2  | 2.51                     | 0.43              |
| 55:B6:9:LEU:HD21    | 55:B6:11:LEU:HD23 | 2.00                     | 0.43              |
| 56:B7:45:ALA:C      | 56:B7:46:VAL:HG23 | 2.39                     | 0.43              |
| 57:B8:8:LYS:HG3     | 57:B8:12:LYS:HE3  | 2.01                     | 0.43              |
| 27:BA:116:C:C2'     | 27:BA:117:G:O5'   | 2.67                     | 0.43              |
| 27:BA:121:G:C8      | 27:BA:121:G:C5'   | 3.01                     | 0.43              |
| 27:BA:1222:C:H2'    | 27:BA:1223:G:C8   | 2.54                     | 0.43              |
| 27:BA:1450(A):C:H2' | 27:BA:1451:C:H6   | 1.83                     | 0.43              |
| 27:BA:1596:A:C3'    | 27:BA:1597:A:H5'  | 2.48                     | 0.43              |
| 27:BA:2298:A:N3     | 27:BA:2299:G:H1'  | 2.33                     | 0.43              |
| 27:BA:2355:C:O5'    | 27:BA:2355:C:H6   | 2.01                     | 0.43              |
| 27:BA:2544:G:C4     | 27:BA:2545:G:C8   | 3.07                     | 0.43              |
| 27:BA:2646:C:C4     | 27:BA:2647:U:C5   | 3.07                     | 0.43              |
| 27:BA:2657:A:C4     | 27:BA:2665:A:C6   | 3.07                     | 0.43              |
| 27:BA:2717:G:H2'    | 27:BA:2718:G:O4'  | 2.18                     | 0.43              |
| 27:BA:2720:U:H5'    | 27:BA:2721:A:OP2  | 2.18                     | 0.43              |
| 27:BA:2823:A:O2'    | 27:BA:2824:C:H5'  | 2.19                     | 0.43              |
| 27:BA:2833:G:HO2'   | 27:BA:2834:G:P    | 2.42                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:319:C:H2'    | 27:BA:320:A:C8     | 2.54                     | 0.43              |
| 27:BA:729:G:H8     | 27:BA:764:A:OP1    | 2.02                     | 0.43              |
| 30:BD:146:GLU:HA   | 30:BD:152:GLY:O    | 2.18                     | 0.43              |
| 30:BD:44:ASN:HB2   | 30:BD:45:ASN:H     | 1.68                     | 0.43              |
| 31:BE:144:ARG:O    | 31:BE:148:GLY:HA2  | 2.19                     | 0.43              |
| 32:BF:113:ALA:O    | 32:BF:116:ASP:HB3  | 2.18                     | 0.43              |
| 32:BF:124:LEU:O    | 32:BF:193:VAL:HA   | 2.19                     | 0.43              |
| 32:BF:160:ASN:ND2  | 32:BF:162:LEU:HB2  | 2.29                     | 0.43              |
| 27:BA:615:G:O2'    | 32:BF:205:ARG:NH2  | 2.51                     | 0.43              |
| 34:BH:156:ALA:CB   | 34:BH:159:GLU:HB3  | 2.48                     | 0.43              |
| 34:BH:54:ARG:HD2   | 34:BH:56:SER:O     | 2.18                     | 0.43              |
| 36:BN:36:GLY:N     | 36:BN:42:TRP:HZ3   | 2.17                     | 0.43              |
| 37:BO:14:THR:HG22  | 37:BO:15:GLY:N     | 2.33                     | 0.43              |
| 37:BO:59:LYS:NZ    | 37:BO:89:ASN:HD21  | 2.17                     | 0.43              |
| 37:BO:75:SER:O     | 37:BO:76:ALA:CB    | 2.67                     | 0.43              |
| 38:BP:123:LEU:O    | 38:BP:123:LEU:HD12 | 2.18                     | 0.43              |
| 38:BP:138:LEU:O    | 38:BP:139:LYS:C    | 2.57                     | 0.43              |
| 39:BQ:109:VAL:HG12 | 39:BQ:110:THR:N    | 2.33                     | 0.43              |
| 39:BQ:27:VAL:HG23  | 39:BQ:137:TYR:CE1  | 2.53                     | 0.43              |
| 39:BQ:36:ALA:C     | 39:BQ:37:LEU:HD22  | 2.38                     | 0.43              |
| 40:BR:87:TYR:O     | 40:BR:88:ARG:C     | 2.56                     | 0.43              |
| 42:BT:109:GLU:O    | 42:BT:112:ARG:HB2  | 2.19                     | 0.43              |
| 42:BT:16:ARG:H     | 42:BT:79:HIS:CD2   | 2.31                     | 0.43              |
| 43:BU:90:VAL:HG11  | 44:BV:40:LEU:CD2   | 2.43                     | 0.43              |
| 44:BV:18:LEU:CD1   | 44:BV:18:LEU:N     | 2.82                     | 0.43              |
| 44:BV:52:VAL:HG22  | 44:BV:55:ALA:CB    | 2.49                     | 0.43              |
| 47:BY:95:LYS:HG2   | 47:BY:100:ALA:CA   | 2.47                     | 0.43              |
| 1:CA:1057:G:C6     | 1:CA:1204:A:C2     | 3.06                     | 0.43              |
| 1:CA:198:G:O2'     | 1:CA:199:G:H5'     | 2.19                     | 0.43              |
| 1:CA:250:A:C1'     | 1:CA:252:U:C6      | 3.02                     | 0.43              |
| 1:CA:276:G:H2'     | 1:CA:277:C:H5'     | 2.01                     | 0.43              |
| 1:CA:340:U:H2'     | 1:CA:341:C:C6      | 2.54                     | 0.43              |
| 1:CA:409:G:H2'     | 1:CA:410:G:O4'     | 2.19                     | 0.43              |
| 1:CA:431:A:H3'     | 1:CA:432:A:H8      | 1.83                     | 0.43              |
| 1:CA:502:G:N1      | 1:CA:544:G:C2      | 2.87                     | 0.43              |
| 1:CA:648:A:N1      | 1:CA:649:G:C6      | 2.86                     | 0.43              |
| 1:CA:741:G:H2'     | 1:CA:742:G:O4'     | 2.18                     | 0.43              |
| 1:CA:862:C:O2'     | 1:CA:874:G:H5''    | 2.18                     | 0.43              |
| 2:CB:119:GLU:O     | 2:CB:122:PHE:HB3   | 2.18                     | 0.43              |
| 2:CB:96:ARG:N      | 2:CB:96:ARG:CD     | 2.74                     | 0.43              |
| 4:CD:60:GLU:O      | 4:CD:63:LYS:N      | 2.52                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:CE:53:LEU:HD12   | 5:CE:53:LEU:N     | 2.26                     | 0.43              |
| 1:CA:737:A:OP1     | 6:CF:91:VAL:HG13  | 2.19                     | 0.43              |
| 7:CG:26:PHE:CD2    | 7:CG:62:PHE:CE1   | 3.07                     | 0.43              |
| 7:CG:77:SER:O      | 7:CG:78:ARG:CB    | 2.66                     | 0.43              |
| 8:CH:6:ILE:HG23    | 8:CH:10:LEU:HD12  | 2.00                     | 0.43              |
| 9:CI:17:VAL:CG1    | 9:CI:81:ILE:HD13  | 2.49                     | 0.43              |
| 1:CA:1147:C:HO2'   | 9:CI:5:TYR:HH     | 1.67                     | 0.43              |
| 12:CL:114:ARG:HH21 | 12:CL:121:LYS:N   | 2.17                     | 0.43              |
| 13:CM:36:LYS:C     | 13:CM:38:GLY:N    | 2.70                     | 0.43              |
| 13:CM:25:ILE:HD11  | 13:CM:66:LEU:HB3  | 1.99                     | 0.43              |
| 13:CM:88:ARG:O     | 13:CM:98:VAL:HG11 | 2.19                     | 0.43              |
| 15:CO:79:ARG:C     | 15:CO:81:LEU:N    | 2.72                     | 0.43              |
| 17:CQ:56:VAL:HB    | 17:CQ:78:GLU:HG3  | 2.00                     | 0.43              |
| 17:CQ:92:ARG:O     | 17:CQ:93:GLN:C    | 2.56                     | 0.43              |
| 1:CA:718:G:N2      | 18:CR:49:LYS:NZ   | 2.54                     | 0.43              |
| 20:CT:16:HIS:CG    | 20:CT:16:HIS:O    | 2.71                     | 0.43              |
| 51:D2:45:SER:O     | 51:D2:46:GLN:NE2  | 2.52                     | 0.43              |
| 27:DA:1049:C:O2'   | 27:DA:1050:A:C8   | 2.65                     | 0.43              |
| 27:DA:1216:G:N1    | 27:DA:1234:U:C2   | 2.87                     | 0.43              |
| 27:DA:1673:U:O4    | 31:DE:129:HIS:HD2 | 2.02                     | 0.43              |
| 27:DA:1815:A:HO2'  | 27:DA:1816:G:C5'  | 2.32                     | 0.43              |
| 27:DA:1858:G:C2    | 27:DA:1883:G:C2   | 3.07                     | 0.43              |
| 27:DA:2056:G:C5    | 27:DA:2577:A:C8   | 3.06                     | 0.43              |
| 27:DA:2287:A:O2'   | 27:DA:2288:A:P    | 2.77                     | 0.43              |
| 27:DA:2302:G:C6    | 27:DA:2303:G:C5   | 3.07                     | 0.43              |
| 27:DA:2542:A:H8    | 27:DA:2544:G:O6   | 2.02                     | 0.43              |
| 27:DA:2022:U:O2'   | 27:DA:2617:C:H5'  | 2.19                     | 0.43              |
| 27:DA:272(E):G:C2  | 27:DA:272(F):C:C2 | 3.07                     | 0.43              |
| 27:DA:760:G:C2'    | 27:DA:761:A:H5'   | 2.48                     | 0.43              |
| 27:DA:856:C:H6     | 27:DA:856:C:H5''  | 1.84                     | 0.43              |
| 28:DB:45:A:H2'     | 28:DB:46:A:C5'    | 2.49                     | 0.43              |
| 29:DC:56:GLN:OE1   | 29:DC:56:GLN:O    | 2.37                     | 0.43              |
| 30:DD:265:PRO:C    | 30:DD:267:SER:H   | 2.22                     | 0.43              |
| 31:DE:111:ARG:O    | 31:DE:112:GLY:O   | 2.36                     | 0.43              |
| 31:DE:150:VAL:O    | 31:DE:152:LYS:N   | 2.52                     | 0.43              |
| 32:DF:132:VAL:O    | 32:DF:133:ASN:O   | 2.37                     | 0.43              |
| 33:DG:126:ASP:C    | 33:DG:128:ARG:N   | 2.71                     | 0.43              |
| 33:DG:18:GLU:O     | 33:DG:22:ARG:HG3  | 2.18                     | 0.43              |
| 33:DG:46:ALA:CA    | 33:DG:51:ARG:HG3  | 2.49                     | 0.43              |
| 34:DH:158:HIS:HE2  | 34:DH:170:ARG:C   | 2.22                     | 0.43              |
| 36:DN:85:ILE:HG12  | 36:DN:89:LYS:HB3  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:DO:11:ALA:CB   | 37:DO:64:ARG:HH21 | 2.30                     | 0.43              |
| 37:DO:53:LYS:O    | 37:DO:54:GLU:C    | 2.57                     | 0.43              |
| 38:DP:64:LYS:HB3  | 57:D8:25:MET:CG   | 2.48                     | 0.43              |
| 39:DQ:47:ILE:HG22 | 39:DQ:48:GLU:N    | 2.34                     | 0.43              |
| 40:DR:11:ASN:OD1  | 40:DR:12:ARG:N    | 2.52                     | 0.43              |
| 40:DR:71:GLN:HE21 | 40:DR:71:GLN:HB2  | 1.63                     | 0.43              |
| 43:DU:5:LYS:HG2   | 43:DU:7:GLY:N     | 2.31                     | 0.43              |
| 43:DU:95:LEU:HA   | 43:DU:95:LEU:HD23 | 1.80                     | 0.43              |
| 43:DU:98:LEU:HD21 | 44:DV:2:PHE:CZ    | 2.54                     | 0.43              |
| 45:DW:26:GLY:N    | 45:DW:71:VAL:HB   | 2.25                     | 0.43              |
| 1:AA:1055:A:C5    | 1:AA:1206:G:C2    | 3.07                     | 0.43              |
| 1:AA:1264:C:O2    | 1:AA:1271:G:N2    | 2.49                     | 0.43              |
| 1:AA:1306:A:N6    | 1:AA:1331:G:O2'   | 2.51                     | 0.43              |
| 1:AA:975:A:H5''   | 1:AA:1365:G:H22   | 1.82                     | 0.43              |
| 1:AA:1375:A:C5    | 1:AA:1376:U:C4    | 3.07                     | 0.43              |
| 1:AA:197:A:N6     | 1:AA:221:C:C5'    | 2.81                     | 0.43              |
| 1:AA:321:A:C6     | 1:AA:333:G:N1     | 2.86                     | 0.43              |
| 1:AA:452:A:H4'    | 16:AP:72:ARG:NH2  | 2.34                     | 0.43              |
| 1:AA:678:U:H2'    | 1:AA:679:C:C6     | 2.53                     | 0.43              |
| 1:AA:681:C:N3     | 1:AA:710:G:C6     | 2.87                     | 0.43              |
| 1:AA:660:G:C2     | 1:AA:746:A:C2     | 3.06                     | 0.43              |
| 1:AA:792:A:H1'    | 1:AA:794:A:N7     | 2.34                     | 0.43              |
| 1:AA:824:C:H2'    | 1:AA:825:G:C8     | 2.53                     | 0.43              |
| 4:AD:68:TYR:O     | 4:AD:69:GLY:C     | 2.57                     | 0.43              |
| 5:AE:91:LEU:HA    | 5:AE:91:LEU:HD12  | 1.80                     | 0.43              |
| 7:AG:155:ARG:O    | 7:AG:156:TRP:CD1  | 2.72                     | 0.43              |
| 7:AG:22:LEU:HD13  | 7:AG:97:GLN:HE21  | 1.82                     | 0.43              |
| 8:AH:127:LEU:HD13 | 8:AH:127:LEU:C    | 2.39                     | 0.43              |
| 8:AH:14:ARG:HG3   | 8:AH:18:ARG:HH11  | 1.84                     | 0.43              |
| 9:AI:49:PRO:HG2   | 9:AI:81:ILE:HG21  | 2.00                     | 0.43              |
| 10:AJ:94:VAL:CG1  | 10:AJ:95:GLU:N    | 2.81                     | 0.43              |
| 11:AK:32:ILE:O    | 11:AK:40:ILE:HG12 | 2.18                     | 0.43              |
| 11:AK:54:ARG:NH1  | 25:AY:39:C:OP1    | 2.52                     | 0.43              |
| 12:AL:7:LEU:HB3   | 17:AQ:32:TYR:CE1  | 2.54                     | 0.43              |
| 13:AM:96:LEU:HD21 | 13:AM:111:LYS:CD  | 2.49                     | 0.43              |
| 14:AN:44:LEU:HG   | 14:AN:45:ARG:N    | 2.34                     | 0.43              |
| 15:AO:62:GLN:HE21 | 15:AO:66:LEU:CD1  | 2.31                     | 0.43              |
| 18:AR:36:ASN:HB2  | 18:AR:39:VAL:HG23 | 2.01                     | 0.43              |
| 1:AA:719:C:O2'    | 18:AR:49:LYS:HB3  | 2.18                     | 0.43              |
| 19:AS:28:LYS:HD3  | 19:AS:28:LYS:HA   | 1.66                     | 0.43              |
| 51:B2:17:SER:H    | 51:B2:67:LYS:NZ   | 2.17                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:B5:49:CYS:C   | 54:B5:50:GLY:O    | 2.57                     | 0.43              |
| 27:BA:1268:A:H2' | 27:BA:1269:A:O4'  | 2.19                     | 0.43              |
| 27:BA:1321:A:C8  | 27:BA:1321:A:H5'' | 2.54                     | 0.43              |
| 27:BA:147:U:H2'  | 27:BA:148:C:H6    | 1.82                     | 0.43              |
| 27:BA:1785:A:N7  | 27:BA:1787:A:C5   | 2.87                     | 0.43              |
| 27:BA:1848:A:C2' | 27:BA:1849:G:C8   | 2.98                     | 0.43              |
| 27:BA:2192:G:C6  | 27:BA:2193:G:N7   | 2.87                     | 0.43              |
| 27:BA:2294:C:OP1 | 41:BS:92:TYR:CE1  | 2.71                     | 0.43              |
| 27:BA:2449:U:O5' | 27:BA:2449:U:H6   | 2.02                     | 0.43              |
| 27:BA:2657:A:C6  | 27:BA:2665:A:C8   | 3.07                     | 0.43              |
| 27:BA:299:A:C4   | 27:BA:322:A:C2    | 3.07                     | 0.43              |
| 27:BA:340:A:C2'  | 27:BA:341:G:O5'   | 2.66                     | 0.43              |
| 27:BA:745:G:C2'  | 27:BA:746:A:H5'   | 2.49                     | 0.43              |
| 27:BA:775:G:C4   | 27:BA:794:G:C8    | 3.06                     | 0.43              |
| 27:BA:864:G:H1'  | 27:BA:914:C:N4    | 2.33                     | 0.43              |
| 30:BD:213:ARG:O  | 30:BD:214:TRP:C   | 2.56                     | 0.43              |
| 30:BD:241:PRO:O  | 30:BD:242:ARG:HD3 | 2.18                     | 0.43              |
| 27:BA:2822:G:OP2 | 31:BE:110:GLY:HA3 | 2.18                     | 0.43              |
| 31:BE:75:VAL:O   | 31:BE:76:ARG:C    | 2.57                     | 0.43              |
| 32:BF:167:ALA:O  | 32:BF:168:ARG:C   | 2.57                     | 0.43              |
| 32:BF:170:LEU:HA | 32:BF:171:PRO:HD3 | 1.69                     | 0.43              |
| 33:BG:45:GLU:HB3 | 33:BG:53:LEU:HG   | 1.99                     | 0.43              |
| 36:BN:91:LEU:CD2 | 36:BN:98:VAL:HG21 | 2.49                     | 0.43              |
| 38:BP:122:PRO:HA | 38:BP:141:ALA:O   | 2.19                     | 0.43              |
| 27:BA:2406:U:C4  | 38:BP:72:PRO:HD2  | 2.54                     | 0.43              |
| 27:BA:1453:U:P   | 40:BR:77:ARG:HH11 | 2.42                     | 0.43              |
| 1:AA:1432:G:OP2  | 42:BT:108:ARG:NH1 | 2.52                     | 0.43              |
| 43:BU:90:VAL:CG1 | 43:BU:91:ASP:N    | 2.73                     | 0.43              |
| 43:BU:91:ASP:C   | 43:BU:91:ASP:OD2  | 2.57                     | 0.43              |
| 45:BW:7:ALA:O    | 45:BW:102:HIS:HA  | 2.19                     | 0.43              |
| 46:BX:18:TYR:O   | 46:BX:20:GLY:N    | 2.52                     | 0.43              |
| 1:CA:1055:A:N1   | 1:CA:1056:U:C2    | 2.87                     | 0.43              |
| 1:CA:1063:C:C5   | 1:CA:1064:G:C4    | 3.06                     | 0.43              |
| 1:CA:1075:C:H4'  | 1:CA:1101:A:N6    | 2.34                     | 0.43              |
| 1:CA:9:G:O2'     | 1:CA:10:A:O4'     | 2.37                     | 0.43              |
| 1:CA:1171:G:O2'  | 1:CA:1172:C:H5'   | 2.19                     | 0.43              |
| 1:CA:1315:U:HO2' | 1:CA:1360:A:H1'   | 1.82                     | 0.43              |
| 1:CA:1409:C:H2'  | 1:CA:1410:G:H8    | 1.84                     | 0.43              |
| 1:CA:362:G:C8    | 1:CA:362:G:H3'    | 2.54                     | 0.43              |
| 1:CA:525:C:H5''  | 12:CL:88:LYS:HZ1  | 1.83                     | 0.43              |
| 1:CA:549:C:H2'   | 1:CA:550:G:O4'    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:671:G:N2     | 1:CA:736:C:C2     | 2.87                     | 0.43              |
| 1:CA:811:C:H5     | 1:CA:812:C:C4     | 2.37                     | 0.43              |
| 1:CA:945:G:H2'    | 1:CA:945:G:N3     | 2.33                     | 0.43              |
| 2:CB:112:VAL:CG1  | 2:CB:153:ARG:HG2  | 2.48                     | 0.43              |
| 2:CB:131:PRO:C    | 2:CB:135:GLN:HG3  | 2.39                     | 0.43              |
| 2:CB:54:THR:HG21  | 2:CB:201:ILE:HD11 | 2.01                     | 0.43              |
| 4:CD:133:VAL:HG21 | 4:CD:138:TYR:CE1  | 2.54                     | 0.43              |
| 7:CG:156:TRP:CG   | 7:CG:156:TRP:OXT  | 2.69                     | 0.43              |
| 8:CH:86:ILE:CG2   | 8:CH:87:SER:N     | 2.79                     | 0.43              |
| 9:CI:23:ASN:N     | 9:CI:23:ASN:HD22  | 2.16                     | 0.43              |
| 1:CA:1151:A:H5'   | 10:CJ:41:PRO:HA   | 2.01                     | 0.43              |
| 1:CA:716:A:H1'    | 11:CK:117:ASN:O   | 2.19                     | 0.43              |
| 13:CM:48:LEU:HB2  | 13:CM:52:GLU:CB   | 2.48                     | 0.43              |
| 15:CO:74:ASP:O    | 15:CO:75:PRO:C    | 2.57                     | 0.43              |
| 19:CS:27:GLU:HB3  | 19:CS:28:LYS:H    | 1.45                     | 0.43              |
| 20:CT:67:ALA:O    | 20:CT:73:HIS:CG   | 2.72                     | 0.43              |
| 20:CT:87:LYS:C    | 20:CT:89:ARG:N    | 2.72                     | 0.43              |
| 24:CX:19:G:C5'    | 24:CX:20:U:C5     | 3.00                     | 0.43              |
| 50:D1:94:LEU:HA   | 50:D1:94:LEU:HD23 | 1.68                     | 0.43              |
| 51:D2:4:SER:HA    | 51:D2:7:ARG:NH1   | 2.05                     | 0.43              |
| 51:D2:4:SER:O     | 51:D2:7:ARG:CG    | 2.67                     | 0.43              |
| 33:DG:104:GLU:HG2 | 53:D4:50:THR:CG2  | 2.49                     | 0.43              |
| 56:D7:47:ARG:O    | 56:D7:48:LYS:HD3  | 2.18                     | 0.43              |
| 27:DA:1191:G:N3   | 27:DA:1192:G:C8   | 2.87                     | 0.43              |
| 27:DA:1362:C:C2'  | 27:DA:1363:C:H5'  | 2.49                     | 0.43              |
| 27:DA:1619:G:H2'  | 27:DA:1620:G:H8   | 1.84                     | 0.43              |
| 27:DA:1649:G:N2   | 27:DA:2009:G:C4   | 2.87                     | 0.43              |
| 27:DA:1650:G:C2   | 27:DA:1651:G:N9   | 2.87                     | 0.43              |
| 27:DA:1651:G:H21  | 27:DA:1652:A:H1'  | 1.84                     | 0.43              |
| 27:DA:1967:C:H2'  | 27:DA:1968:G:H5'  | 2.00                     | 0.43              |
| 27:DA:1651:G:H1   | 27:DA:2006:C:H42  | 1.67                     | 0.43              |
| 27:DA:211:A:H2'   | 27:DA:212:G:C8    | 2.54                     | 0.43              |
| 27:DA:2253:G:O2'  | 27:DA:2254:C:H5'  | 2.18                     | 0.43              |
| 27:DA:2346:A:C5   | 27:DA:2383:G:C6   | 3.07                     | 0.43              |
| 27:DA:2548:G:C2'  | 27:DA:2549:G:O5'  | 2.67                     | 0.43              |
| 27:DA:2582:G:H2'  | 27:DA:2583:G:H8   | 1.83                     | 0.43              |
| 27:DA:2611:U:O2   | 54:D5:3:LYS:HE3   | 2.18                     | 0.43              |
| 27:DA:746:A:C8    | 27:DA:2612:C:OP1  | 2.72                     | 0.43              |
| 27:DA:2616:C:H2'  | 27:DA:2617:C:H6   | 1.84                     | 0.43              |
| 27:DA:2657:A:O2'  | 34:DH:160:LYS:HE3 | 2.19                     | 0.43              |
| 27:DA:2759:G:N2   | 34:DH:139:GLN:OE1 | 2.51                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2774:C:H2'   | 27:DA:2775:A:O4'   | 2.19                     | 0.43              |
| 27:DA:2778:A:H4'   | 27:DA:2779:U:OP2   | 2.19                     | 0.43              |
| 27:DA:2787:C:H2'   | 27:DA:2787:C:O2    | 2.18                     | 0.43              |
| 27:DA:2816:C:O2    | 27:DA:2883:A:O2'   | 2.36                     | 0.43              |
| 27:DA:289:A:H5''   | 27:DA:290:G:OP2    | 2.19                     | 0.43              |
| 27:DA:28:A:H2'     | 27:DA:29:U:H5'     | 2.01                     | 0.43              |
| 27:DA:345:A:O2'    | 27:DA:347:A:N7     | 2.51                     | 0.43              |
| 27:DA:400:G:O5'    | 27:DA:400:G:H8     | 2.01                     | 0.43              |
| 27:DA:529:A:C5     | 27:DA:2042:A:C2    | 3.07                     | 0.43              |
| 27:DA:743:G:H2'    | 27:DA:744:G:H5'    | 1.99                     | 0.43              |
| 27:DA:784:A:C8     | 27:DA:792:G:C5     | 3.07                     | 0.43              |
| 28:DB:28:C:N4      | 28:DB:29:A:N6      | 2.67                     | 0.43              |
| 27:DA:1816:G:C6    | 30:DD:37:LEU:HD11  | 2.53                     | 0.43              |
| 31:DE:116:VAL:CG2  | 31:DE:122:PHE:HB2  | 2.48                     | 0.43              |
| 31:DE:116:VAL:HG23 | 31:DE:122:PHE:CG   | 2.53                     | 0.43              |
| 32:DF:160:ASN:C    | 32:DF:162:LEU:H    | 2.22                     | 0.43              |
| 34:DH:169:VAL:O    | 34:DH:169:VAL:HG13 | 2.18                     | 0.43              |
| 34:DH:94:TYR:CD2   | 34:DH:107:VAL:HG12 | 2.53                     | 0.43              |
| 38:DP:88:LEU:HD13  | 38:DP:114:ILE:HD11 | 2.00                     | 0.43              |
| 27:DA:1246:A:OP1   | 38:DP:18:ARG:HD3   | 2.19                     | 0.43              |
| 43:DU:52:ARG:HD3   | 43:DU:55:ARG:NE    | 2.33                     | 0.43              |
| 43:DU:94:ASN:C     | 43:DU:94:ASN:OD1   | 2.57                     | 0.43              |
| 44:DV:19:LYS:HG2   | 44:DV:94:LEU:O     | 2.19                     | 0.43              |
| 47:DY:18:GLY:O     | 47:DY:20:TYR:N     | 2.51                     | 0.43              |
| 48:DZ:138:VAL:HG12 | 48:DZ:139:ASP:N    | 2.34                     | 0.43              |
| 1:AA:1067:A:O3'    | 1:AA:1094:G:OP1    | 2.37                     | 0.43              |
| 1:AA:1157:A:O4'    | 1:AA:1158:C:C2     | 2.72                     | 0.43              |
| 1:AA:1054:C:OP1    | 1:AA:1198:G:OP2    | 2.36                     | 0.43              |
| 1:AA:236:G:O2'     | 1:AA:237:C:H5'     | 2.19                     | 0.43              |
| 1:AA:483:C:OP2     | 1:AA:484:G:H3'     | 2.18                     | 0.43              |
| 1:AA:443:C:C2      | 1:AA:492:G:C2      | 3.07                     | 0.43              |
| 1:AA:751:U:C4'     | 15:AO:24:SER:CA    | 2.92                     | 0.43              |
| 1:AA:816:A:HO2'    | 1:AA:817:C:P       | 2.41                     | 0.43              |
| 1:AA:818:G:H3'     | 1:AA:819:A:H5'     | 1.99                     | 0.43              |
| 1:AA:828:A:H61     | 1:AA:858:G:H2'     | 1.84                     | 0.43              |
| 1:AA:876:G:C4      | 1:AA:877:C:C5      | 3.07                     | 0.43              |
| 2:AB:47:THR:O      | 2:AB:51:LEU:HG     | 2.18                     | 0.43              |
| 4:AD:98:GLU:HA     | 4:AD:103:ASN:HD22  | 1.84                     | 0.43              |
| 5:AE:16:THR:OG1    | 5:AE:17:ALA:N      | 2.51                     | 0.43              |
| 7:AG:152:ALA:HB1   | 7:AG:155:ARG:HH12  | 1.84                     | 0.43              |
| 5:AE:151:LEU:HD21  | 8:AH:66:GLY:HA2    | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AH:44:PHE:HB3    | 8:AH:80:ILE:HG12   | 1.99                     | 0.43              |
| 9:AI:37:PHE:HB3    | 9:AI:40:LEU:HB2    | 2.01                     | 0.43              |
| 9:AI:6:GLY:HA2     | 9:AI:83:ARG:HG2    | 2.01                     | 0.43              |
| 9:AI:81:ILE:C      | 9:AI:83:ARG:H      | 2.22                     | 0.43              |
| 10:AJ:32:ALA:CB    | 10:AJ:75:ILE:HD11  | 2.49                     | 0.43              |
| 15:AO:34:LEU:C     | 15:AO:36:ILE:N     | 2.72                     | 0.43              |
| 19:AS:79:THR:O     | 19:AS:80:TYR:CB    | 2.67                     | 0.43              |
| 20:AT:14:LYS:HA    | 20:AT:17:ARG:NE    | 2.33                     | 0.43              |
| 52:B3:53:LEU:O     | 52:B3:54:VAL:HG23  | 2.19                     | 0.43              |
| 27:BA:2742:C:P     | 58:B9:35:ARG:NH1   | 2.92                     | 0.43              |
| 27:BA:52:A:C5      | 27:BA:118:A:C2     | 3.07                     | 0.43              |
| 27:BA:1207:C:H2'   | 27:BA:1208:C:C6    | 2.53                     | 0.43              |
| 27:BA:1221(A):C:C2 | 27:BA:1229:G:N2    | 2.87                     | 0.43              |
| 27:BA:1467:C:C4    | 27:BA:1546:C:O2    | 2.72                     | 0.43              |
| 27:BA:1645:G:H4'   | 27:BA:1646:C:C6    | 2.53                     | 0.43              |
| 27:BA:1654:A:OP2   | 40:BR:3:HIS:CB     | 2.65                     | 0.43              |
| 27:BA:2245:U:H5'   | 27:BA:2246:G:H5'   | 2.00                     | 0.43              |
| 27:BA:2462:U:H2'   | 27:BA:2463:C:C6    | 2.54                     | 0.43              |
| 27:BA:10:G:O6      | 27:BA:2629:A:H8    | 2.02                     | 0.43              |
| 27:BA:2704:C:H2'   | 27:BA:2705:A:O4'   | 2.19                     | 0.43              |
| 27:BA:2838:G:C1'   | 40:BR:45:ARG:NH1   | 2.82                     | 0.43              |
| 27:BA:477:A:H2'    | 27:BA:478:A:O4'    | 2.19                     | 0.43              |
| 27:BA:528:A:O5'    | 27:BA:528:A:H8     | 2.01                     | 0.43              |
| 27:BA:624:C:H41    | 38:BP:107:LYS:HZ3  | 1.66                     | 0.43              |
| 27:BA:833:U:H2'    | 27:BA:834:C:C6     | 2.52                     | 0.43              |
| 27:BA:947:G:N2     | 27:BA:971:C:C2     | 2.87                     | 0.43              |
| 30:BD:4:LYS:HE3    | 30:BD:21:PHE:CE1   | 2.54                     | 0.43              |
| 30:BD:31:LYS:O     | 30:BD:32:SER:C     | 2.57                     | 0.43              |
| 31:BE:146:THR:HA   | 31:BE:147:PRO:C    | 2.39                     | 0.43              |
| 31:BE:24:THR:HG21  | 31:BE:188:VAL:HB   | 2.01                     | 0.43              |
| 32:BF:21:ALA:O     | 32:BF:24:LEU:N     | 2.49                     | 0.43              |
| 32:BF:82:ILE:O     | 32:BF:82:ILE:HG12  | 2.18                     | 0.43              |
| 32:BF:8:GLN:HB2    | 32:BF:124:LEU:HD11 | 2.00                     | 0.43              |
| 32:BF:89:VAL:CG1   | 32:BF:90:PHE:N     | 2.77                     | 0.43              |
| 33:BG:138:GLN:HB2  | 33:BG:155:MET:HE2  | 2.01                     | 0.43              |
| 33:BG:55:LYS:HZ3   | 33:BG:148:MET:C    | 2.23                     | 0.43              |
| 38:BP:126:VAL:HG12 | 38:BP:148:LEU:HD11 | 2.00                     | 0.43              |
| 40:BR:21:TYR:CZ    | 40:BR:43:GLU:HG2   | 2.54                     | 0.43              |
| 40:BR:79:LEU:CA    | 40:BR:83:ILE:HG13  | 2.32                     | 0.43              |
| 40:BR:87:TYR:O     | 40:BR:90:ARG:N     | 2.52                     | 0.43              |
| 42:BT:23:ARG:NH2   | 42:BT:120:ARG:HD3  | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:BU:12:ARG:HB3  | 43:BU:15:LYS:NZ   | 2.33                     | 0.43              |
| 43:BU:88:ILE:C    | 43:BU:90:VAL:N    | 2.73                     | 0.43              |
| 27:BA:751:A:C4'   | 45:BW:90:ARG:HG2  | 2.48                     | 0.43              |
| 1:CA:1053:G:C2    | 1:CA:1199:U:C4    | 3.07                     | 0.43              |
| 1:CA:1348:U:H2'   | 1:CA:1349:A:C8    | 2.47                     | 0.43              |
| 1:CA:1349:A:H2'   | 1:CA:1350:A:H8    | 1.84                     | 0.43              |
| 1:CA:232:G:HO2'   | 1:CA:263:A:H2     | 1.67                     | 0.43              |
| 1:CA:363:A:O2'    | 1:CA:364:A:H5'    | 2.19                     | 0.43              |
| 1:CA:442:C:H3'    | 1:CA:442:C:H6     | 1.84                     | 0.43              |
| 1:CA:563:A:C2'    | 1:CA:567:G:C8     | 3.02                     | 0.43              |
| 1:CA:747:C:C5     | 1:CA:748:C:N3     | 2.87                     | 0.43              |
| 1:CA:876:G:OP1    | 8:CH:14:ARG:NH1   | 2.52                     | 0.43              |
| 1:CA:878:G:C6     | 1:CA:879:C:C4     | 3.07                     | 0.43              |
| 1:CA:989:C:H2'    | 1:CA:990:C:H6     | 1.83                     | 0.43              |
| 2:CB:116:GLU:HA   | 2:CB:119:GLU:HB2  | 2.00                     | 0.43              |
| 2:CB:189:ASP:N    | 2:CB:189:ASP:OD1  | 2.51                     | 0.43              |
| 4:CD:111:ALA:HA   | 4:CD:116:GLN:OE1  | 2.19                     | 0.43              |
| 4:CD:170:VAL:CG1  | 4:CD:174:LEU:HB2  | 2.49                     | 0.43              |
| 1:CA:27:G:C4'     | 4:CD:209:ARG:OXT  | 2.67                     | 0.43              |
| 5:CE:45:PHE:C     | 5:CE:45:PHE:CD1   | 2.92                     | 0.43              |
| 6:CF:41:GLU:HB2   | 6:CF:62:TRP:CE3   | 2.54                     | 0.43              |
| 6:CF:22:GLU:OE1   | 6:CF:84:ASN:HB2   | 2.19                     | 0.43              |
| 8:CH:29:SER:HB3   | 8:CH:32:LYS:CG    | 2.46                     | 0.43              |
| 10:CJ:53:PRO:HG2  | 10:CJ:54:PHE:H    | 1.84                     | 0.43              |
| 10:CJ:89:ASP:C    | 10:CJ:90:LEU:HD12 | 2.40                     | 0.43              |
| 11:CK:120:ARG:HB2 | 11:CK:120:ARG:HE  | 1.66                     | 0.43              |
| 1:CA:33:A:N3      | 12:CL:29:PHE:HE2  | 2.17                     | 0.43              |
| 12:CL:38:ARG:CZ   | 12:CL:38:ARG:CB   | 2.96                     | 0.43              |
| 12:CL:3:THR:O     | 12:CL:4:ILE:C     | 2.57                     | 0.43              |
| 13:CM:60:VAL:HG12 | 13:CM:66:LEU:HD21 | 2.01                     | 0.43              |
| 14:CN:57:ARG:HG2  | 14:CN:58:LYS:H    | 1.81                     | 0.43              |
| 1:CA:754:C:O4'    | 15:CO:69:TYR:CD1  | 2.72                     | 0.43              |
| 1:CA:473:G:C5'    | 16:CP:81:ARG:HE   | 2.32                     | 0.43              |
| 17:CQ:22:LEU:HD11 | 17:CQ:39:SER:OG   | 2.19                     | 0.43              |
| 20:CT:40:ALA:C    | 20:CT:42:GLN:N    | 2.72                     | 0.43              |
| 20:CT:63:ILE:HD13 | 20:CT:80:ARG:HB2  | 2.01                     | 0.43              |
| 23:CW:17:G:H1'    | 23:CW:56:G:N2     | 2.34                     | 0.43              |
| 23:CW:56:G:C2'    | 23:CW:57:A:C5'    | 2.96                     | 0.43              |
| 25:CY:14:A:H1'    | 25:CY:21:A:N1     | 2.33                     | 0.43              |
| 25:CY:37:U:H2'    | 25:CY:38:U:C5'    | 2.48                     | 0.43              |
| 25:CY:42:G:H8     | 25:CY:42:G:OP2    | 2.01                     | 0.43              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 51:D2:23:LYS:O   | 51:D2:25:VAL:N     | 2.52                     | 0.43              |
| 51:D2:39:ALA:O   | 51:D2:42:GLY:N     | 2.45                     | 0.43              |
| 45:DW:35:ILE:O   | 54:D5:28:PRO:HG3   | 2.18                     | 0.43              |
| 54:D5:37:LYS:HG3 | 54:D5:38:ALA:N     | 2.33                     | 0.43              |
| 56:D7:46:VAL:CG1 | 56:D7:48:LYS:NZ    | 2.82                     | 0.43              |
| 58:D9:9:ARG:HG3  | 58:D9:9:ARG:H      | 1.44                     | 0.43              |
| 27:DA:1022:G:O2' | 27:DA:1023:U:O5'   | 2.36                     | 0.43              |
| 27:DA:1210:A:OP1 | 27:DA:1212:G:H5'   | 2.18                     | 0.43              |
| 27:DA:1333:C:O2' | 27:DA:1334:G:H5'   | 2.19                     | 0.43              |
| 27:DA:1484:G:N2  | 27:DA:1505:C:N4    | 2.67                     | 0.43              |
| 27:DA:1611:C:H5' | 27:DA:1611:C:C6    | 2.52                     | 0.43              |
| 27:DA:1668:A:H2  | 27:DA:1670:C:N3    | 2.17                     | 0.43              |
| 27:DA:1827:C:H5' | 27:DA:1972:A:OP2   | 2.19                     | 0.43              |
| 27:DA:1926:U:O2' | 27:DA:1928:A:N7    | 2.37                     | 0.43              |
| 27:DA:1968:G:H2' | 27:DA:1969:A:H5''  | 1.98                     | 0.43              |
| 27:DA:1984:G:O2' | 27:DA:1985:G:C5'   | 2.62                     | 0.43              |
| 27:DA:860:U:C2   | 27:DA:2268:A:C8    | 3.07                     | 0.43              |
| 27:DA:2301:C:C6  | 27:DA:2301:C:H3'   | 2.52                     | 0.43              |
| 27:DA:2340:G:H2' | 27:DA:2341:G:H8    | 1.82                     | 0.43              |
| 27:DA:2363:C:C2  | 27:DA:2364:C:C5    | 3.07                     | 0.43              |
| 27:DA:2417:C:H2' | 27:DA:2418:A:H8    | 1.84                     | 0.43              |
| 27:DA:456:C:O2'  | 27:DA:457:A:OP2    | 2.32                     | 0.43              |
| 27:DA:55:G:N3    | 27:DA:56:A:C8      | 2.87                     | 0.43              |
| 27:DA:663:G:C6   | 27:DA:664:C:C4     | 3.07                     | 0.43              |
| 27:DA:948:G:H2'  | 27:DA:949:C:H6     | 1.81                     | 0.43              |
| 28:DB:20:C:H2'   | 28:DB:21:G:C5'     | 2.49                     | 0.43              |
| 28:DB:70:C:O2'   | 28:DB:71:C:H5'     | 2.18                     | 0.43              |
| 30:DD:130:ALA:C  | 30:DD:131:LEU:HD12 | 2.39                     | 0.43              |
| 30:DD:52:ARG:HB2 | 30:DD:53:PHE:CE2   | 2.54                     | 0.43              |
| 31:DE:16:ARG:O   | 31:DE:18:ASP:N     | 2.43                     | 0.43              |
| 31:DE:65:GLY:O   | 31:DE:67:PHE:O     | 2.37                     | 0.43              |
| 33:DG:166:ASP:O  | 33:DG:170:ARG:N    | 2.50                     | 0.43              |
| 33:DG:27:ASN:C   | 33:DG:29:TRP:H     | 2.21                     | 0.43              |
| 34:DH:64:LEU:O   | 34:DH:68:THR:CB    | 2.67                     | 0.43              |
| 36:DN:98:VAL:O   | 36:DN:102:ALA:HB2  | 2.18                     | 0.43              |
| 38:DP:105:LEU:O  | 38:DP:106:LEU:CB   | 2.54                     | 0.43              |
| 42:DT:125:ARG:O  | 42:DT:128:GLU:CG   | 2.67                     | 0.43              |
| 43:DU:65:ILE:O   | 43:DU:68:ALA:HB3   | 2.19                     | 0.43              |
| 44:DV:5:VAL:HG23 | 44:DV:37:VAL:HG21  | 1.97                     | 0.43              |
| 45:DW:70:TYR:C   | 45:DW:70:TYR:CD2   | 2.92                     | 0.43              |
| 48:DZ:95:VAL:CG1 | 48:DZ:96:GLU:N     | 2.82                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1015:A:N3     | 1:AA:1218:C:O2'   | 2.50                     | 0.42              |
| 1:AA:1084:G:OP1    | 1:AA:1086:U:N3    | 2.52                     | 0.42              |
| 1:AA:1087:G:C2     | 1:AA:1088:G:C5    | 3.07                     | 0.42              |
| 1:AA:1239:A:H1'    | 1:AA:1241:G:C5    | 2.53                     | 0.42              |
| 1:AA:1240:U:H3'    | 1:AA:1241:G:C5'   | 2.48                     | 0.42              |
| 1:AA:1385:G:O2'    | 1:AA:1386:G:H5'   | 2.19                     | 0.42              |
| 1:AA:1413:A:C2     | 1:AA:1488:G:C2    | 3.07                     | 0.42              |
| 1:AA:266:G:O2'     | 1:AA:267:C:OP2    | 2.31                     | 0.42              |
| 1:AA:390:C:H6      | 1:AA:390:C:O5'    | 2.01                     | 0.42              |
| 1:AA:402:G:C2'     | 1:AA:403:C:H5'    | 2.48                     | 0.42              |
| 1:AA:420:U:C2      | 1:AA:422:C:N3     | 2.87                     | 0.42              |
| 1:AA:495:A:O2'     | 1:AA:496:A:O5'    | 2.35                     | 0.42              |
| 1:AA:758:G:C5'     | 1:AA:880:C:H1'    | 2.49                     | 0.42              |
| 2:AB:130:ARG:HA    | 2:AB:131:PRO:HD2  | 1.86                     | 0.42              |
| 5:AE:126:ARG:CG    | 5:AE:126:ARG:HH11 | 2.29                     | 0.42              |
| 1:AA:1346:A:C5     | 7:AG:10:ARG:CZ    | 3.02                     | 0.42              |
| 7:AG:24:THR:O      | 7:AG:27:ILE:N     | 2.51                     | 0.42              |
| 8:AH:97:VAL:C      | 8:AH:99:GLU:H     | 2.23                     | 0.42              |
| 9:AI:70:LYS:HA     | 9:AI:73:GLN:HE21  | 1.83                     | 0.42              |
| 10:AJ:25:GLU:H     | 10:AJ:25:GLU:HG2  | 1.67                     | 0.42              |
| 10:AJ:34:VAL:CG1   | 10:AJ:73:ASP:O    | 2.66                     | 0.42              |
| 12:AL:2:PRO:C      | 12:AL:6:GLN:HE21  | 2.21                     | 0.42              |
| 13:AM:15:VAL:C     | 13:AM:17:VAL:H    | 2.22                     | 0.42              |
| 17:AQ:56:VAL:CG2   | 17:AQ:81:ARG:HG3  | 2.49                     | 0.42              |
| 18:AR:37:VAL:HG12  | 18:AR:78:LEU:HB3  | 2.01                     | 0.42              |
| 20:AT:100:ILE:HD12 | 20:AT:100:ILE:N   | 2.34                     | 0.42              |
| 49:B0:37:LEU:HD11  | 49:B0:61:ALA:N    | 2.34                     | 0.42              |
| 27:BA:1113:U:H2'   | 27:BA:1113:U:O2   | 2.18                     | 0.42              |
| 27:BA:1249:U:C6    | 27:BA:1249:U:C5'  | 2.90                     | 0.42              |
| 27:BA:143:G:H1'    | 46:BX:37:THR:CG2  | 2.43                     | 0.42              |
| 27:BA:1555:G:C2    | 27:BA:1556:C:C4   | 3.07                     | 0.42              |
| 27:BA:1689:A:H62   | 27:BA:1698:A:H2   | 1.66                     | 0.42              |
| 27:BA:1822:G:N1    | 27:BA:1823:G:C5   | 2.87                     | 0.42              |
| 27:BA:19:C:O5'     | 27:BA:19:C:H6     | 2.01                     | 0.42              |
| 27:BA:2283:C:C3'   | 27:BA:2284:C:H5'  | 2.47                     | 0.42              |
| 27:BA:2371:G:C4'   | 55:B6:45:LYS:HB3  | 2.49                     | 0.42              |
| 27:BA:2590:A:H2'   | 27:BA:2591:C:C6   | 2.54                     | 0.42              |
| 27:BA:2657:A:H2'   | 27:BA:2658:C:H5'  | 2.01                     | 0.42              |
| 27:BA:266:G:C2'    | 27:BA:267:C:O5'   | 2.67                     | 0.42              |
| 27:BA:271(Y):U:O2' | 27:BA:271(Z):C:P  | 2.77                     | 0.42              |
| 27:BA:2831:G:H1'   | 27:BA:2883:A:H2'  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:687:C:C2    | 27:BA:788:A:H5'   | 2.54                     | 0.42              |
| 27:BA:693:C:C2'   | 27:BA:694:U:H5'   | 2.49                     | 0.42              |
| 27:BA:73:A:O2'    | 27:BA:74:A:P      | 2.77                     | 0.42              |
| 28:BB:66:A:C2'    | 28:BB:67:G:OP2    | 2.67                     | 0.42              |
| 29:BC:193:ILE:O   | 29:BC:194:ARG:C   | 2.57                     | 0.42              |
| 30:BD:31:LYS:HB3  | 30:BD:35:LYS:CG   | 2.45                     | 0.42              |
| 30:BD:68:LYS:CE   | 30:BD:70:TRP:NE1  | 2.82                     | 0.42              |
| 32:BF:37:VAL:HG12 | 32:BF:41:LEU:HD12 | 2.01                     | 0.42              |
| 33:BG:51:ARG:HA   | 33:BG:53:LEU:HD23 | 2.01                     | 0.42              |
| 34:BH:100:GLY:C   | 34:BH:102:ALA:H   | 2.21                     | 0.42              |
| 38:BP:82:GLY:HA2  | 38:BP:113:LYS:O   | 2.19                     | 0.42              |
| 41:BS:61:ASN:OD1  | 41:BS:64:GLU:CB   | 2.67                     | 0.42              |
| 42:BT:16:ARG:HH22 | 42:BT:82:LEU:CD1  | 2.32                     | 0.42              |
| 43:BU:92:ARG:CZ   | 44:BV:11:GLN:HB2  | 2.48                     | 0.42              |
| 46:BX:12:VAL:HG11 | 46:BX:27:THR:HG23 | 2.01                     | 0.42              |
| 1:CA:1038:C:H6    | 1:CA:1038:C:O5'   | 2.02                     | 0.42              |
| 1:CA:122:G:O3'    | 1:CA:312:C:H4'    | 2.19                     | 0.42              |
| 1:CA:1238:A:C8    | 1:CA:1303:C:H1'   | 2.54                     | 0.42              |
| 1:CA:1429:C:O2'   | 1:CA:1430:C:H5'   | 2.19                     | 0.42              |
| 1:CA:161:A:O2'    | 1:CA:162:A:H5'    | 2.19                     | 0.42              |
| 1:CA:252:U:C4     | 1:CA:253:U:O4     | 2.72                     | 0.42              |
| 1:CA:407:G:C4     | 1:CA:408:A:C8     | 3.06                     | 0.42              |
| 1:CA:453:A:C5     | 1:CA:454:C:C5     | 3.07                     | 0.42              |
| 1:CA:686:U:N3     | 1:CA:703:G:N2     | 2.64                     | 0.42              |
| 2:CB:236:TYR:CD2  | 2:CB:239:VAL:HG21 | 2.54                     | 0.42              |
| 2:CB:57:PHE:O     | 2:CB:61:LEU:N     | 2.42                     | 0.42              |
| 6:CF:36:ARG:O     | 6:CF:65:VAL:HB    | 2.19                     | 0.42              |
| 8:CH:83:ILE:O     | 8:CH:83:ILE:HG12  | 2.18                     | 0.42              |
| 8:CH:86:ILE:CG2   | 8:CH:87:SER:H     | 2.26                     | 0.42              |
| 10:CJ:16:LEU:HD13 | 10:CJ:70:ARG:NE   | 2.33                     | 0.42              |
| 10:CJ:32:ALA:CB   | 10:CJ:76:ASN:CB   | 2.92                     | 0.42              |
| 12:CL:25:LYS:C    | 12:CL:27:ALA:H    | 2.23                     | 0.42              |
| 12:CL:3:THR:CG2   | 12:CL:6:GLN:HB2   | 2.47                     | 0.42              |
| 14:CN:26:ARG:HG3  | 14:CN:27:CYS:H    | 1.84                     | 0.42              |
| 14:CN:42:ILE:H    | 14:CN:42:ILE:HG12 | 1.54                     | 0.42              |
| 14:CN:26:ARG:CZ   | 14:CN:47:LEU:HD21 | 2.49                     | 0.42              |
| 15:CO:87:ILE:CG2  | 15:CO:88:ARG:H    | 2.12                     | 0.42              |
| 16:CP:18:ARG:HG3  | 16:CP:35:LYS:HE3  | 2.01                     | 0.42              |
| 16:CP:18:ARG:O    | 16:CP:19:ILE:C    | 2.57                     | 0.42              |
| 17:CQ:11:VAL:HG11 | 17:CQ:88:TYR:CD2  | 2.54                     | 0.42              |
| 17:CQ:83:ASP:O    | 17:CQ:87:LYS:HG2  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:CR:32:ARG:CA   | 18:CR:69:THR:HG21  | 2.45                     | 0.42              |
| 25:CY:7:A:N6      | 25:CY:48:C:C4      | 2.82                     | 0.42              |
| 39:DQ:85:LYS:HG3  | 49:D0:7:LEU:CG     | 2.49                     | 0.42              |
| 52:D3:47:VAL:O    | 52:D3:50:VAL:HG22  | 2.18                     | 0.42              |
| 57:D8:37:SER:OG   | 57:D8:39:LYS:HB3   | 2.19                     | 0.42              |
| 57:D8:7:HIS:C     | 57:D8:7:HIS:ND1    | 2.72                     | 0.42              |
| 27:DA:1499:C:C2'  | 27:DA:1500:G:H5'   | 2.48                     | 0.42              |
| 27:DA:14:A:C6     | 27:DA:526:A:C2     | 3.06                     | 0.42              |
| 27:DA:151:C:H2'   | 27:DA:152:G:H5'    | 1.98                     | 0.42              |
| 27:DA:13:A:C4     | 27:DA:15:G:O6      | 2.72                     | 0.42              |
| 27:DA:1897:G:N1   | 27:DA:1898:U:C2    | 2.87                     | 0.42              |
| 27:DA:203:C:C3'   | 27:DA:204:A:H5''   | 2.45                     | 0.42              |
| 27:DA:2199:A:C6   | 27:DA:2200:C:C2    | 3.06                     | 0.42              |
| 27:DA:2439:A:C8   | 27:DA:2439:A:C5'   | 3.02                     | 0.42              |
| 27:DA:2454:G:C2'  | 27:DA:2455:G:H5'   | 2.49                     | 0.42              |
| 27:DA:2536:G:H2'  | 27:DA:2537:U:C6    | 2.53                     | 0.42              |
| 27:DA:2570:G:H2'  | 27:DA:2571:C:O4'   | 2.18                     | 0.42              |
| 27:DA:2637:U:H4'  | 31:DE:44:TYR:CD1   | 2.54                     | 0.42              |
| 27:DA:2839:G:C5   | 27:DA:2840:C:C4    | 3.07                     | 0.42              |
| 27:DA:2850:A:C4   | 27:DA:2851:A:C8    | 3.07                     | 0.42              |
| 27:DA:2879:C:H4'  | 27:DA:2880:C:C5    | 2.54                     | 0.42              |
| 27:DA:223:A:H2    | 27:DA:407:G:N3     | 2.17                     | 0.42              |
| 27:DA:484:C:O2'   | 27:DA:485:C:H5'    | 2.19                     | 0.42              |
| 27:DA:593:G:C6    | 27:DA:594:U:C4     | 3.07                     | 0.42              |
| 27:DA:678:C:H2'   | 27:DA:679:C:C6     | 2.54                     | 0.42              |
| 27:DA:732:C:C4    | 27:DA:733:G:C6     | 3.07                     | 0.42              |
| 27:DA:992:C:H6    | 27:DA:992:C:H3'    | 1.84                     | 0.42              |
| 28:DB:4:C:C2      | 28:DB:118:G:C2     | 3.07                     | 0.42              |
| 28:DB:51:G:H5'    | 28:DB:52:A:OP2     | 2.19                     | 0.42              |
| 29:DC:36:LYS:HA   | 29:DC:36:LYS:NZ    | 2.34                     | 0.42              |
| 31:DE:179:GLU:HA  | 31:DE:179:GLU:OE1  | 2.19                     | 0.42              |
| 32:DF:178:PRO:HB3 | 32:DF:201:VAL:HG11 | 2.01                     | 0.42              |
| 33:DG:172:LEU:O   | 33:DG:176:LEU:HG   | 2.19                     | 0.42              |
| 27:DA:2746:U:O4'  | 34:DH:139:GLN:HA   | 2.19                     | 0.42              |
| 36:DN:35:ARG:NH2  | 36:DN:108:PRO:HG2  | 2.34                     | 0.42              |
| 36:DN:3:THR:C     | 36:DN:5:VAL:N      | 2.72                     | 0.42              |
| 37:DO:12:ASP:OD1  | 37:DO:86:ILE:CD1   | 2.67                     | 0.42              |
| 37:DO:101:PRO:CG  | 42:DT:67:SER:HB3   | 2.48                     | 0.42              |
| 43:DU:60:LEU:HD13 | 43:DU:60:LEU:C     | 2.39                     | 0.42              |
| 45:DW:17:VAL:O    | 45:DW:18:ARG:C     | 2.56                     | 0.42              |
| 45:DW:17:VAL:O    | 45:DW:20:VAL:HB    | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:DW:84:ARG:N     | 45:DW:96:ILE:O     | 2.39                     | 0.42              |
| 47:DY:76:CYS:C     | 47:DY:78:ALA:N     | 2.72                     | 0.42              |
| 48:DZ:156:LEU:HD22 | 48:DZ:162:LEU:HD12 | 2.01                     | 0.42              |
| 1:AA:1125:U:C2'    | 1:AA:1126:U:OP2    | 2.67                     | 0.42              |
| 1:AA:1157:A:H1'    | 1:AA:1181:G:H21    | 1.84                     | 0.42              |
| 1:AA:1310:G:O2'    | 1:AA:1311:G:H5'    | 2.18                     | 0.42              |
| 1:AA:1343:G:H1'    | 9:AI:121:ARG:HH12  | 1.84                     | 0.42              |
| 1:AA:20:U:C2'      | 1:AA:21:G:H5'      | 2.49                     | 0.42              |
| 1:AA:917:G:C2      | 1:AA:918:A:C4      | 3.07                     | 0.42              |
| 2:AB:8:LYS:O       | 2:AB:11:LEU:HB2    | 2.19                     | 0.42              |
| 3:AC:113:ALA:O     | 3:AC:116:VAL:N     | 2.52                     | 0.42              |
| 4:AD:9:CYS:N       | 4:AD:22:LYS:NZ     | 2.57                     | 0.42              |
| 6:AF:82:ARG:HD2    | 6:AF:82:ARG:HA     | 1.91                     | 0.42              |
| 1:AA:939:G:C5'     | 7:AG:102:ARG:NH1   | 2.77                     | 0.42              |
| 9:AI:113:LYS:H     | 9:AI:119:ALA:HA    | 1.84                     | 0.42              |
| 10:AJ:63:PHE:HA    | 14:AN:59:ALA:H     | 1.82                     | 0.42              |
| 11:AK:44:SER:H     | 11:AK:47:VAL:HB    | 1.84                     | 0.42              |
| 12:AL:2:PRO:O      | 12:AL:3:THR:C      | 2.58                     | 0.42              |
| 13:AM:17:VAL:O     | 13:AM:21:TYR:HD1   | 2.01                     | 0.42              |
| 14:AN:24:CYS:N     | 14:AN:33:VAL:CG1   | 2.82                     | 0.42              |
| 15:AO:42:HIS:O     | 15:AO:42:HIS:CG    | 2.72                     | 0.42              |
| 16:AP:31:LYS:HG2   | 16:AP:32:TYR:N     | 2.34                     | 0.42              |
| 50:B1:90:ILE:HD13  | 50:B1:90:ILE:HA    | 1.82                     | 0.42              |
| 56:B7:29:LYS:O     | 56:B7:33:ARG:N     | 2.46                     | 0.42              |
| 58:B9:3:VAL:O      | 58:B9:4:ARG:HB3    | 2.19                     | 0.42              |
| 27:BA:1049:C:N4    | 27:BA:1111:A:C2    | 2.87                     | 0.42              |
| 27:BA:1158:C:H1'   | 52:B3:32:GLN:HG3   | 2.01                     | 0.42              |
| 27:BA:1268:A:C2    | 27:BA:2013:A:C4    | 3.07                     | 0.42              |
| 27:BA:1404:C:C2'   | 27:BA:1404:C:O2    | 2.62                     | 0.42              |
| 27:BA:1558:A:O2'   | 27:BA:1559:G:OP2   | 2.30                     | 0.42              |
| 27:BA:1612:C:H2'   | 27:BA:1613:G:O5'   | 2.19                     | 0.42              |
| 27:BA:1645:G:O3'   | 27:BA:1646:C:H6    | 2.01                     | 0.42              |
| 27:BA:2018:G:H2'   | 27:BA:2019:A:C8    | 2.54                     | 0.42              |
| 27:BA:235:U:H2'    | 27:BA:236:C:C6     | 2.54                     | 0.42              |
| 27:BA:2785:C:H2'   | 27:BA:2786:U:O4'   | 2.19                     | 0.42              |
| 27:BA:2842:G:H2'   | 27:BA:2843:G:O4'   | 2.20                     | 0.42              |
| 27:BA:31:C:C2'     | 27:BA:32:C:H5'     | 2.49                     | 0.42              |
| 27:BA:415:A:H2'    | 27:BA:415:A:N3     | 2.35                     | 0.42              |
| 27:BA:445:C:C4     | 27:BA:446:G:C6     | 3.07                     | 0.42              |
| 27:BA:642:G:H21    | 27:BA:646:A:H2     | 1.66                     | 0.42              |
| 27:BA:723:G:C6     | 27:BA:724:U:C4     | 3.06                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:962:G:H2'   | 27:BA:963:U:H6     | 1.84                     | 0.42              |
| 28:BB:88:C:C4     | 28:BB:89:G:C6      | 3.08                     | 0.42              |
| 30:BD:31:LYS:O    | 30:BD:33:LEU:N     | 2.53                     | 0.42              |
| 30:BD:85:ASP:CB   | 30:BD:92:ILE:HG23  | 2.49                     | 0.42              |
| 32:BF:187:VAL:O   | 32:BF:189:THR:N    | 2.52                     | 0.42              |
| 32:BF:63:LYS:HG3  | 32:BF:75:HIS:O     | 2.19                     | 0.42              |
| 33:BG:172:LEU:O   | 33:BG:173:LEU:C    | 2.56                     | 0.42              |
| 33:BG:16:ARG:CB   | 33:BG:17:PRO:CD    | 2.97                     | 0.42              |
| 35:BI:69:LYS:O    | 35:BI:73:GLU:CB    | 2.67                     | 0.42              |
| 38:BP:105:LEU:N   | 38:BP:105:LEU:CD2  | 2.77                     | 0.42              |
| 27:BA:1242:A:N1   | 38:BP:8:PRO:HG3    | 2.35                     | 0.42              |
| 40:BR:28:LEU:CD2  | 40:BR:114:VAL:HG12 | 2.48                     | 0.42              |
| 40:BR:37:THR:HA   | 40:BR:110:PRO:O    | 2.19                     | 0.42              |
| 41:BS:54:LEU:HD13 | 41:BS:58:LEU:CB    | 2.49                     | 0.42              |
| 45:BW:12:ILE:CD1  | 45:BW:17:VAL:HG12  | 2.48                     | 0.42              |
| 1:CA:102:G:C4     | 1:CA:103:C:C5      | 3.07                     | 0.42              |
| 1:CA:1137:C:C4'   | 1:CA:1138:G:N2     | 2.73                     | 0.42              |
| 1:CA:1305:G:HO2'  | 1:CA:1306:A:P      | 2.41                     | 0.42              |
| 1:CA:1311:G:N1    | 1:CA:1312:G:C5     | 2.87                     | 0.42              |
| 1:CA:1310:G:C2    | 1:CA:1328:C:N3     | 2.86                     | 0.42              |
| 1:CA:1331:G:OP2   | 13:CM:23:TYR:CD2   | 2.72                     | 0.42              |
| 1:CA:922:G:N3     | 1:CA:1398:A:H2     | 2.17                     | 0.42              |
| 1:CA:144:G:H2'    | 1:CA:145:G:O4'     | 2.20                     | 0.42              |
| 1:CA:1462:G:O2'   | 1:CA:1463:C:H5'    | 2.19                     | 0.42              |
| 1:CA:157:G:H2'    | 1:CA:158:G:H8      | 1.84                     | 0.42              |
| 1:CA:184:G:C4'    | 1:CA:224:C:H4'     | 2.49                     | 0.42              |
| 1:CA:54:C:N4      | 1:CA:353:A:OP2     | 2.52                     | 0.42              |
| 1:CA:972:C:O2'    | 1:CA:973:G:H5'     | 2.19                     | 0.42              |
| 3:CC:140:ARG:HG3  | 3:CC:140:ARG:HH11  | 1.83                     | 0.42              |
| 3:CC:184:TYR:HD1  | 3:CC:201:TYR:HE2   | 1.67                     | 0.42              |
| 3:CC:73:PRO:O     | 3:CC:75:VAL:N      | 2.51                     | 0.42              |
| 4:CD:79:PHE:C     | 4:CD:79:PHE:CD2    | 2.92                     | 0.42              |
| 6:CF:3:ARG:NH1    | 6:CF:38:GLU:OE1    | 2.52                     | 0.42              |
| 8:CH:114:THR:N    | 8:CH:117:GLY:O     | 2.51                     | 0.42              |
| 9:CI:125:TYR:C    | 9:CI:125:TYR:CD2   | 2.93                     | 0.42              |
| 10:CJ:32:ALA:H    | 10:CJ:76:ASN:HD22  | 1.67                     | 0.42              |
| 10:CJ:84:GLN:CD   | 10:CJ:84:GLN:N     | 2.73                     | 0.42              |
| 11:CK:124:LYS:HB2 | 11:CK:124:LYS:HE3  | 1.54                     | 0.42              |
| 12:CL:87:VAL:O    | 12:CL:88:LYS:C     | 2.56                     | 0.42              |
| 15:CO:67:LEU:HA   | 15:CO:67:LEU:HD23  | 1.81                     | 0.42              |
| 16:CP:68:ASP:HA   | 16:CP:71:ARG:CD    | 2.49                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 19:CS:22:LEU:O      | 19:CS:26:GLY:CA    | 2.67                     | 0.42              |
| 19:CS:49:ILE:O      | 19:CS:60:VAL:HG12  | 2.19                     | 0.42              |
| 19:CS:79:THR:O      | 19:CS:80:TYR:CB    | 2.67                     | 0.42              |
| 24:CX:62:C:H2'      | 24:CX:62:C:O2      | 2.17                     | 0.42              |
| 24:CX:63:G:O2'      | 24:CX:64:G:H5'     | 2.19                     | 0.42              |
| 52:D3:46:ASN:O      | 52:D3:47:VAL:C     | 2.58                     | 0.42              |
| 52:D3:7:LYS:CE      | 52:D3:32:GLN:NE2   | 2.82                     | 0.42              |
| 27:DA:2016:U:H1'    | 54:D5:6:VAL:HG13   | 2.00                     | 0.42              |
| 55:D6:17:LYS:HA     | 55:D6:17:LYS:HD3   | 1.66                     | 0.42              |
| 27:DA:1206:G:O2'    | 27:DA:1207:C:C5'   | 2.67                     | 0.42              |
| 27:DA:1327:C:H2'    | 27:DA:1328:G:C8    | 2.55                     | 0.42              |
| 27:DA:134:C:H2'     | 27:DA:135:G:O4'    | 2.18                     | 0.42              |
| 27:DA:1381:G:C2'    | 27:DA:1382:G:H5'   | 2.49                     | 0.42              |
| 27:DA:1394:U:C4     | 27:DA:1395:A:C5    | 3.07                     | 0.42              |
| 27:DA:1429:G:C4     | 27:DA:1568:G:C2    | 3.06                     | 0.42              |
| 27:DA:1441:G:O2'    | 27:DA:1442:G:H5'   | 2.18                     | 0.42              |
| 27:DA:1787:A:N3     | 27:DA:1787:A:H2'   | 2.34                     | 0.42              |
| 27:DA:2060:A:O2'    | 27:DA:2061:G:P     | 2.77                     | 0.42              |
| 27:DA:2113:U:O2'    | 27:DA:2114:A:P     | 2.77                     | 0.42              |
| 27:DA:2231:C:H2'    | 27:DA:2232:U:C6    | 2.54                     | 0.42              |
| 27:DA:2351:G:O2'    | 27:DA:2366:A:N6    | 2.52                     | 0.42              |
| 27:DA:2432:A:H2'    | 27:DA:2433:A:C8    | 2.54                     | 0.42              |
| 27:DA:2520:C:N3     | 27:DA:2521:C:C4    | 2.87                     | 0.42              |
| 27:DA:2647:U:H2'    | 27:DA:2648:C:H6    | 1.84                     | 0.42              |
| 27:DA:2696:U:H2'    | 27:DA:2697:G:C8    | 2.54                     | 0.42              |
| 27:DA:2772:C:C2     | 27:DA:2773:C:C5    | 3.07                     | 0.42              |
| 27:DA:280:C:C5      | 27:DA:281:G:N7     | 2.86                     | 0.42              |
| 27:DA:355:G:H2'     | 27:DA:356:G:O4'    | 2.19                     | 0.42              |
| 27:DA:411:G:H4'     | 27:DA:412:A:O5'    | 2.19                     | 0.42              |
| 27:DA:530:G:C5      | 27:DA:2022:U:H5''  | 2.54                     | 0.42              |
| 27:DA:533:G:H5'     | 43:DU:24:TYR:HD2   | 1.84                     | 0.42              |
| 27:DA:541:C:C4      | 27:DA:542:C:N4     | 2.87                     | 0.42              |
| 27:DA:614(A):U:H5'' | 27:DA:614(B):G:OP1 | 2.19                     | 0.42              |
| 27:DA:697:C:N4      | 27:DA:698:C:N4     | 2.67                     | 0.42              |
| 27:DA:909:A:N1      | 27:DA:912:C:H1'    | 2.34                     | 0.42              |
| 30:DD:176:ARG:CG    | 30:DD:177:LEU:N    | 2.82                     | 0.42              |
| 30:DD:144:ALA:HB3   | 30:DD:192:THR:CG2  | 2.48                     | 0.42              |
| 30:DD:245:PRO:O     | 30:DD:246:PRO:C    | 2.56                     | 0.42              |
| 31:DE:119:ARG:HG2   | 31:DE:160:TYR:CG   | 2.54                     | 0.42              |
| 32:DF:202:PHE:O     | 32:DF:205:ARG:N    | 2.37                     | 0.42              |
| 32:DF:46:ARG:O      | 32:DF:48:THR:N     | 2.46                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DF:47:GLY:O     | 32:DF:94:PRO:HA    | 2.19                     | 0.42              |
| 33:DG:122:PRO:HG2  | 33:DG:123:ASN:OD1  | 2.19                     | 0.42              |
| 34:DH:107:VAL:HG23 | 34:DH:107:VAL:O    | 2.19                     | 0.42              |
| 34:DH:16:SER:HB2   | 34:DH:27:LYS:HB2   | 2.01                     | 0.42              |
| 35:DI:123:LEU:HD23 | 35:DI:142:VAL:HG12 | 2.01                     | 0.42              |
| 35:DI:4:ILE:HD11   | 35:DI:44:LEU:HD12  | 2.00                     | 0.42              |
| 36:DN:86:PRO:HG2   | 36:DN:89:LYS:HB2   | 2.01                     | 0.42              |
| 39:DQ:111:GLU:OE2  | 39:DQ:133:ARG:NH2  | 2.52                     | 0.42              |
| 41:DS:61:ASN:O     | 41:DS:62:LYS:CB    | 2.68                     | 0.42              |
| 43:DU:65:ILE:HG23  | 43:DU:106:PHE:HZ   | 1.85                     | 0.42              |
| 43:DU:98:LEU:O     | 43:DU:101:ARG:O    | 2.37                     | 0.42              |
| 44:DV:79:VAL:O     | 44:DV:79:VAL:HG22  | 2.19                     | 0.42              |
| 27:DA:494:G:H4'    | 45:DW:6:ILE:HG22   | 2.00                     | 0.42              |
| 1:AA:1030(A):G:H1' | 1:AA:1031:G:N2     | 2.33                     | 0.42              |
| 1:AA:1036:G:H3'    | 1:AA:1037:C:C6     | 2.54                     | 0.42              |
| 1:AA:1245:A:C6     | 1:AA:1293:G:N1     | 2.87                     | 0.42              |
| 1:AA:1279:A:H4'    | 1:AA:1280:A:OP1    | 2.19                     | 0.42              |
| 1:AA:1359:C:O2'    | 1:AA:1361:G:N7     | 2.52                     | 0.42              |
| 1:AA:279:A:O2'     | 1:AA:280:C:P       | 2.77                     | 0.42              |
| 1:AA:293:G:N3      | 1:AA:293:G:H2'     | 2.35                     | 0.42              |
| 1:AA:34:C:H6       | 1:AA:34:C:O5'      | 2.02                     | 0.42              |
| 1:AA:443:C:N3      | 1:AA:491:G:O6      | 2.52                     | 0.42              |
| 1:AA:506:G:H2'     | 1:AA:507:C:H6      | 1.84                     | 0.42              |
| 1:AA:965:A:O2'     | 1:AA:966:G:O5'     | 2.34                     | 0.42              |
| 1:AA:992:U:H1'     | 1:AA:993:G:N3      | 2.33                     | 0.42              |
| 3:AC:119:ARG:O     | 3:AC:119:ARG:HG2   | 2.18                     | 0.42              |
| 3:AC:11:ARG:HA     | 3:AC:14:ILE:HG23   | 2.01                     | 0.42              |
| 4:AD:121:VAL:HG12  | 4:AD:134:ASP:HA    | 2.01                     | 0.42              |
| 1:AA:406:G:H5'     | 4:AD:5:ILE:HD13    | 2.01                     | 0.42              |
| 6:AF:92:LYS:O      | 6:AF:93:SER:C      | 2.58                     | 0.42              |
| 7:AG:109:ASN:HD22  | 7:AG:109:ASN:N     | 2.17                     | 0.42              |
| 8:AH:26:VAL:CG2    | 8:AH:27:PRO:N      | 2.82                     | 0.42              |
| 8:AH:56:LYS:HB3    | 8:AH:58:TYR:HE1    | 1.84                     | 0.42              |
| 8:AH:69:ARG:HH12   | 8:AH:76:PRO:CA     | 2.24                     | 0.42              |
| 12:AL:74:LEU:CD2   | 12:AL:104:ALA:HB2  | 2.49                     | 0.42              |
| 16:AP:58:TYR:CD1   | 16:AP:59:TRP:N     | 2.87                     | 0.42              |
| 1:AA:1320:C:H41    | 19:AS:37:ARG:HB3   | 1.84                     | 0.42              |
| 23:AW:35:G:C6      | 23:AW:36:A:C5      | 3.08                     | 0.42              |
| 23:AW:67:C:H2'     | 23:AW:68:C:H6      | 1.83                     | 0.42              |
| 23:AW:6:U:C3'      | 23:AW:7:A:C5'      | 2.91                     | 0.42              |
| 24:AX:23:C:O2'     | 24:AX:24:U:H5'     | 2.19                     | 0.42              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 49:B0:55:ARG:HG3    | 49:B0:55:ARG:H    | 1.57                     | 0.42              |
| 51:B2:2:LYS:O       | 51:B2:6:VAL:HG23  | 2.19                     | 0.42              |
| 53:B4:40:ILE:HA     | 53:B4:57:ILE:HG21 | 1.99                     | 0.42              |
| 55:B6:44:ARG:HA     | 55:B6:44:ARG:HD3  | 1.75                     | 0.42              |
| 57:B8:11:LYS:N      | 57:B8:60:LEU:HD21 | 2.34                     | 0.42              |
| 27:BA:1028:A:H2'    | 27:BA:1029:A:C8   | 2.53                     | 0.42              |
| 27:BA:1171:G:C5'    | 27:BA:1173:G:OP2  | 2.67                     | 0.42              |
| 27:BA:1179:C:O2'    | 27:BA:1180:C:C5'  | 2.66                     | 0.42              |
| 27:BA:1204:A:N1     | 27:BA:1241:A:C2   | 2.86                     | 0.42              |
| 27:BA:1328:G:H2'    | 27:BA:1330:C:N4   | 2.34                     | 0.42              |
| 27:BA:1367:A:C5     | 27:BA:1368:G:H1'  | 2.54                     | 0.42              |
| 27:BA:1385:G:O3'    | 27:BA:1396:U:C5   | 2.72                     | 0.42              |
| 27:BA:1418:G:OP1    | 27:BA:1588:C:O2'  | 2.37                     | 0.42              |
| 27:BA:1491:G:C5     | 27:BA:1500:G:N2   | 2.88                     | 0.42              |
| 27:BA:1509(B):A:H2' | 27:BA:1510:G:O4'  | 2.18                     | 0.42              |
| 27:BA:1558:A:N3     | 27:BA:1558:A:O4'  | 2.53                     | 0.42              |
| 27:BA:1554:A:C2     | 27:BA:1634:A:N6   | 2.87                     | 0.42              |
| 27:BA:1654:A:OP2    | 40:BR:3:HIS:CG    | 2.72                     | 0.42              |
| 27:BA:1829:A:H2'    | 27:BA:1830:C:C5'  | 2.49                     | 0.42              |
| 27:BA:2092:U:HO2'   | 27:BA:2093:G:P    | 2.41                     | 0.42              |
| 27:BA:2248:C:H3'    | 27:BA:2249:U:H6   | 1.85                     | 0.42              |
| 27:BA:2345:G:OP2    | 55:B6:39:TYR:HD1  | 2.02                     | 0.42              |
| 27:BA:2631:G:C6     | 27:BA:2632:A:N7   | 2.88                     | 0.42              |
| 27:BA:2642:G:C2     | 27:BA:2773:C:N3   | 2.87                     | 0.42              |
| 27:BA:527:C:O2      | 27:BA:527:C:O4'   | 2.36                     | 0.42              |
| 27:BA:675:A:C6      | 27:BA:676:A:N6    | 2.87                     | 0.42              |
| 27:BA:817:C:HO2'    | 27:BA:818:G:H5'   | 1.83                     | 0.42              |
| 27:BA:996:A:HO2'    | 27:BA:997:G:P     | 2.42                     | 0.42              |
| 30:BD:13:ARG:HA     | 30:BD:16:MET:HE3  | 2.01                     | 0.42              |
| 30:BD:72:LYS:CB     | 30:BD:97:TYR:CE2  | 3.02                     | 0.42              |
| 31:BE:23:VAL:HA     | 31:BE:184:VAL:O   | 2.19                     | 0.42              |
| 31:BE:55:ASN:HD22   | 31:BE:55:ASN:HA   | 1.54                     | 0.42              |
| 32:BF:128:ALA:O     | 32:BF:129:PHE:C   | 2.58                     | 0.42              |
| 32:BF:178:PRO:HG2   | 32:BF:179:GLU:CD  | 2.39                     | 0.42              |
| 33:BG:145:THR:HG1   | 33:BG:147:ASP:CG  | 2.21                     | 0.42              |
| 33:BG:135:LEU:HB2   | 33:BG:155:MET:HG3 | 2.01                     | 0.42              |
| 33:BG:58:GLN:O      | 33:BG:62:LEU:HD12 | 2.19                     | 0.42              |
| 33:BG:71:THR:O      | 33:BG:88:ILE:O    | 2.37                     | 0.42              |
| 35:BI:129:THR:O     | 35:BI:130:TYR:HB2 | 2.18                     | 0.42              |
| 35:BI:37:VAL:HG12   | 35:BI:38:LEU:H    | 1.85                     | 0.42              |
| 35:BI:98:ALA:O      | 35:BI:102:SER:N   | 2.45                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BN:93:THR:O    | 36:BN:94:HIS:CB   | 2.68                     | 0.42              |
| 37:BO:3:GLN:HB2   | 37:BO:4:PRO:HD2   | 2.02                     | 0.42              |
| 38:BP:16:ARG:HG3  | 38:BP:17:LYS:H    | 1.84                     | 0.42              |
| 38:BP:59:LEU:CA   | 38:BP:61:ARG:NH2  | 2.77                     | 0.42              |
| 40:BR:33:ARG:HE   | 40:BR:115:GLU:CB  | 2.32                     | 0.42              |
| 28:BB:50:G:OP1    | 41:BS:63:THR:HG23 | 2.19                     | 0.42              |
| 42:BT:23:ARG:HB2  | 42:BT:24:PRO:HD2  | 1.99                     | 0.42              |
| 42:BT:65:LYS:CG   | 42:BT:66:VAL:N    | 2.80                     | 0.42              |
| 44:BV:62:LEU:HD11 | 44:BV:95:LEU:HB2  | 2.02                     | 0.42              |
| 45:BW:15:ARG:HA   | 45:BW:18:ARG:HB2  | 2.01                     | 0.42              |
| 45:BW:90:ARG:CB   | 45:BW:90:ARG:NH1  | 2.68                     | 0.42              |
| 45:BW:92:ARG:O    | 45:BW:93:ALA:CB   | 2.67                     | 0.42              |
| 1:CA:1182:G:H5'   | 1:CA:1184:G:H5''  | 2.01                     | 0.42              |
| 1:CA:1198:G:H2'   | 1:CA:1199:U:O4'   | 2.19                     | 0.42              |
| 1:CA:1216:G:N2    | 1:CA:1217:C:N3    | 2.67                     | 0.42              |
| 1:CA:1402:C:O5'   | 1:CA:1402:C:H6    | 2.03                     | 0.42              |
| 1:CA:153:C:N3     | 1:CA:169:C:N4     | 2.67                     | 0.42              |
| 1:CA:189(C):C:N3  | 1:CA:189(I):G:C2  | 2.88                     | 0.42              |
| 1:CA:22:G:H2'     | 1:CA:23:C:C6      | 2.55                     | 0.42              |
| 1:CA:342:C:H2'    | 1:CA:343:U:C6     | 2.54                     | 0.42              |
| 1:CA:428:G:H4'    | 1:CA:429:U:O5'    | 2.18                     | 0.42              |
| 1:CA:643:C:H2'    | 1:CA:644:G:H8     | 1.85                     | 0.42              |
| 1:CA:577:G:C4     | 1:CA:816:A:C2     | 3.06                     | 0.42              |
| 1:CA:983:A:C2'    | 1:CA:983:A:N3     | 2.79                     | 0.42              |
| 4:CD:120:LEU:HA   | 4:CD:120:LEU:HD23 | 1.83                     | 0.42              |
| 4:CD:17:VAL:HG13  | 4:CD:18:LYS:N     | 2.34                     | 0.42              |
| 4:CD:31:CYS:O     | 4:CD:31:CYS:SG    | 2.78                     | 0.42              |
| 4:CD:39:PRO:HB2   | 4:CD:44:GLY:HA2   | 2.01                     | 0.42              |
| 4:CD:72:GLU:O     | 4:CD:73:ARG:C     | 2.57                     | 0.42              |
| 4:CD:88:VAL:HG12  | 4:CD:90:GLY:H     | 1.83                     | 0.42              |
| 5:CE:40:ARG:HG2   | 5:CE:40:ARG:NH1   | 2.34                     | 0.42              |
| 8:CH:10:LEU:HD13  | 8:CH:85:ARG:CG    | 2.48                     | 0.42              |
| 9:CI:2:GLU:O      | 9:CI:2:GLU:CD     | 2.58                     | 0.42              |
| 10:CJ:51:ARG:NE   | 10:CJ:60:ARG:O    | 2.52                     | 0.42              |
| 10:CJ:90:LEU:N    | 10:CJ:91:PRO:HD3  | 2.34                     | 0.42              |
| 12:CL:8:VAL:HG11  | 17:CQ:36:ILE:HG21 | 2.01                     | 0.42              |
| 15:CO:78:TYR:O    | 15:CO:81:LEU:HB3  | 2.20                     | 0.42              |
| 15:CO:83:GLU:C    | 15:CO:86:GLY:H    | 2.20                     | 0.42              |
| 17:CQ:60:ILE:HG23 | 17:CQ:61:GLU:O    | 2.19                     | 0.42              |
| 18:CR:65:ILE:O    | 18:CR:66:LEU:C    | 2.58                     | 0.42              |
| 24:CX:66:C:H2'    | 24:CX:67:C:O4'    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:D0:49:LYS:CB    | 49:D0:80:HIS:HB3   | 2.46                     | 0.42              |
| 55:D6:34:LEU:HD23  | 55:D6:34:LEU:HA    | 1.84                     | 0.42              |
| 38:DP:50:ARG:HD3   | 57:D8:7:HIS:CD2    | 2.54                     | 0.42              |
| 58:D9:22:ARG:HB3   | 58:D9:23:VAL:H     | 1.61                     | 0.42              |
| 27:DA:1215:G:H1    | 27:DA:1235:G:H1'   | 1.84                     | 0.42              |
| 27:DA:1286:A:C2'   | 27:DA:1288:U:OP2   | 2.68                     | 0.42              |
| 27:DA:1669:A:C2'   | 27:DA:1670:C:H5'   | 2.49                     | 0.42              |
| 27:DA:1685:C:C2'   | 27:DA:1686:C:H5''  | 2.47                     | 0.42              |
| 27:DA:1688:U:O2    | 27:DA:1700:A:H5'   | 2.19                     | 0.42              |
| 27:DA:1773:A:O2'   | 27:DA:1774:C:H5'   | 2.20                     | 0.42              |
| 27:DA:1932:A:H2'   | 27:DA:1933:G:O4'   | 2.18                     | 0.42              |
| 27:DA:2195:C:O2    | 27:DA:2195:C:H2'   | 2.19                     | 0.42              |
| 27:DA:2255:G:O2'   | 27:DA:2256:G:H5'   | 2.18                     | 0.42              |
| 27:DA:2399:G:C2    | 27:DA:2418:A:C2    | 3.06                     | 0.42              |
| 27:DA:2420:C:OP2   | 57:D8:33:ASN:O     | 2.36                     | 0.42              |
| 27:DA:957:A:N1     | 27:DA:2459:A:C8    | 2.87                     | 0.42              |
| 27:DA:2468:G:N2    | 27:DA:2481:G:C2'   | 2.83                     | 0.42              |
| 27:DA:1953:A:C2    | 27:DA:2549:G:N3    | 2.87                     | 0.42              |
| 27:DA:2650:U:H2'   | 27:DA:2651:C:C6    | 2.53                     | 0.42              |
| 27:DA:2748:A:H62   | 27:DA:2754:U:H3    | 1.65                     | 0.42              |
| 27:DA:2793:G:O2'   | 27:DA:2794:C:P     | 2.78                     | 0.42              |
| 27:DA:486:C:O2     | 27:DA:495:G:C2     | 2.73                     | 0.42              |
| 27:DA:475:U:O4'    | 27:DA:509:C:C2     | 2.73                     | 0.42              |
| 27:DA:542:C:H2'    | 27:DA:542:C:O2     | 2.18                     | 0.42              |
| 27:DA:574:C:HO2'   | 27:DA:2055:C:H5    | 1.65                     | 0.42              |
| 27:DA:596:G:C2     | 27:DA:597:U:C2     | 3.07                     | 0.42              |
| 27:DA:746:A:C1'    | 27:DA:748:G:H21    | 2.32                     | 0.42              |
| 28:DB:71:C:C2'     | 28:DB:72:G:H5'     | 2.49                     | 0.42              |
| 29:DC:68:LEU:HD21  | 29:DC:180:PHE:CB   | 2.49                     | 0.42              |
| 30:DD:198:ASN:CG   | 30:DD:198:ASN:O    | 2.58                     | 0.42              |
| 27:DA:1491:G:H5'   | 30:DD:99:ASP:OD1   | 2.19                     | 0.42              |
| 31:DE:44:TYR:O     | 31:DE:45:THR:C     | 2.57                     | 0.42              |
| 31:DE:54:GLN:HA    | 31:DE:72:VAL:CG1   | 2.48                     | 0.42              |
| 31:DE:7:VAL:O      | 31:DE:26:ILE:HA    | 2.18                     | 0.42              |
| 27:DA:2749:A:C1'   | 34:DH:63:SER:OG    | 2.68                     | 0.42              |
| 35:DI:121:LYS:HG3  | 35:DI:121:LYS:O    | 2.19                     | 0.42              |
| 27:DA:1138:G:O2'   | 36:DN:102:ALA:O    | 2.38                     | 0.42              |
| 36:DN:34:LEU:HD11  | 36:DN:120:LEU:CD2  | 2.27                     | 0.42              |
| 38:DP:125:VAL:O    | 38:DP:125:VAL:HG23 | 2.20                     | 0.42              |
| 39:DQ:109:VAL:HG13 | 39:DQ:113:GLN:CB   | 2.49                     | 0.42              |
| 27:DA:962:G:H21    | 39:DQ:83:MET:HE1   | 1.85                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:DU:117:GLN:O    | 43:DU:118:GLY:C   | 2.57                     | 0.42              |
| 44:DV:18:LEU:O     | 44:DV:19:LYS:HB3  | 2.18                     | 0.42              |
| 44:DV:58:VAL:O     | 44:DV:59:ALA:HB2  | 2.20                     | 0.42              |
| 44:DV:62:LEU:CD2   | 44:DV:94:LEU:HA   | 2.49                     | 0.42              |
| 47:DY:47:LYS:CD    | 47:DY:47:LYS:N    | 2.80                     | 0.42              |
| 47:DY:67:LEU:HG    | 47:DY:67:LEU:O    | 2.19                     | 0.42              |
| 48:DZ:19:ARG:C     | 48:DZ:21:GLY:N    | 2.72                     | 0.42              |
| 1:AA:1086:U:C2'    | 1:AA:1087:G:H5'   | 2.49                     | 0.42              |
| 1:AA:1226:C:OP1    | 19:AS:81:ARG:NH1  | 2.53                     | 0.42              |
| 1:AA:1288:A:H1'    | 1:AA:1352:C:O2'   | 2.19                     | 0.42              |
| 1:AA:1338:G:C6     | 1:AA:1339:A:C6    | 3.07                     | 0.42              |
| 1:AA:18:C:H2'      | 1:AA:19:C:C6      | 2.54                     | 0.42              |
| 1:AA:227:G:O2'     | 1:AA:228:A:H5'    | 2.19                     | 0.42              |
| 1:AA:27:G:H2'      | 1:AA:28:G:H8      | 1.85                     | 0.42              |
| 1:AA:403:C:HO2'    | 1:AA:404:U:H5'    | 1.83                     | 0.42              |
| 1:AA:445:G:N1      | 1:AA:446:G:C5     | 2.87                     | 0.42              |
| 1:AA:592:G:C2      | 1:AA:593:G:C8     | 3.07                     | 0.42              |
| 2:AB:102:LEU:N     | 2:AB:102:LEU:HD12 | 2.34                     | 0.42              |
| 6:AF:32:ASN:C      | 6:AF:34:GLY:H     | 2.23                     | 0.42              |
| 6:AF:2:ARG:HB2     | 6:AF:4:TYR:CE2    | 2.54                     | 0.42              |
| 8:AH:44:PHE:CE2    | 8:AH:109:ILE:HG22 | 2.52                     | 0.42              |
| 8:AH:4:ASP:OD1     | 8:AH:7:ALA:CB     | 2.67                     | 0.42              |
| 9:AI:69:GLY:C      | 9:AI:73:GLN:HG3   | 2.40                     | 0.42              |
| 10:AJ:26:ALA:CA    | 10:AJ:29:ARG:HH21 | 2.32                     | 0.42              |
| 11:AK:117:ASN:HD22 | 11:AK:117:ASN:HA  | 1.68                     | 0.42              |
| 12:AL:9:ARG:HB2    | 12:AL:10:LYS:H    | 1.57                     | 0.42              |
| 17:AQ:93:GLN:HB3   | 17:AQ:93:GLN:HE21 | 1.63                     | 0.42              |
| 1:AA:1320:C:O2     | 19:AS:72:GLY:HA3  | 2.20                     | 0.42              |
| 25:AY:42:G:C2      | 25:AY:43:C:H1'    | 2.54                     | 0.42              |
| 25:AY:43:C:OP2     | 25:AY:44:U:O4     | 2.37                     | 0.42              |
| 27:BA:1044:G:O2'   | 27:BA:1111:A:N6   | 2.52                     | 0.42              |
| 27:BA:1109:C:C5'   | 27:BA:1110:G:OP2  | 2.67                     | 0.42              |
| 27:BA:1447:G:C2    | 27:BA:1465:G:C4   | 3.07                     | 0.42              |
| 27:BA:1466:G:N2    | 27:BA:1547:C:N3   | 2.67                     | 0.42              |
| 27:BA:1469:A:N6    | 27:BA:1470:G:C6   | 2.88                     | 0.42              |
| 27:BA:1465:G:H5'   | 27:BA:1528:A:H1'  | 2.01                     | 0.42              |
| 27:BA:1466:G:H2'   | 27:BA:1547:C:C4   | 2.54                     | 0.42              |
| 27:BA:2008:C:H2'   | 27:BA:2009:G:H8   | 1.84                     | 0.42              |
| 27:BA:2048:G:H2'   | 27:BA:2049:G:O5'  | 2.19                     | 0.42              |
| 27:BA:2073:C:H42   | 27:BA:2436:G:H1   | 1.68                     | 0.42              |
| 25:AY:18:G:C6      | 27:BA:2112:G:N7   | 2.87                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2145:C:H3'  | 27:BA:2145:C:C6    | 2.54                     | 0.42              |
| 27:BA:2158:A:O2'  | 27:BA:2159:G:C8    | 2.68                     | 0.42              |
| 27:BA:268:C:H42   | 27:BA:424:G:H1     | 1.66                     | 0.42              |
| 27:BA:271(V):G:C2 | 27:BA:271(W):G:H1' | 2.54                     | 0.42              |
| 27:BA:2870:C:C2'  | 27:BA:2871:C:C5'   | 2.85                     | 0.42              |
| 27:BA:495:G:C6    | 27:BA:496:G:C5     | 3.08                     | 0.42              |
| 27:BA:704:G:O2'   | 27:BA:726:G:N2     | 2.32                     | 0.42              |
| 27:BA:89:G:H3'    | 27:BA:90:U:C5'     | 2.46                     | 0.42              |
| 28:BB:15:A:H5'    | 28:BB:16:G:C8      | 2.55                     | 0.42              |
| 28:BB:60:C:H2'    | 28:BB:61:G:H8      | 1.84                     | 0.42              |
| 29:BC:128:GLY:O   | 29:BC:130:ILE:N    | 2.43                     | 0.42              |
| 29:BC:45:ALA:HA   | 29:BC:210:ARG:HA   | 2.01                     | 0.42              |
| 30:BD:16:MET:O    | 30:BD:17:THR:HG23  | 2.19                     | 0.42              |
| 30:BD:174:ILE:O   | 30:BD:174:ILE:HG22 | 2.17                     | 0.42              |
| 31:BE:52:LEU:HA   | 31:BE:53:PRO:HD3   | 1.85                     | 0.42              |
| 31:BE:69:LYS:HZ2  | 31:BE:89:ASP:HA    | 1.83                     | 0.42              |
| 32:BF:114:VAL:O   | 32:BF:115:ALA:C    | 2.58                     | 0.42              |
| 32:BF:117:ARG:NH1 | 32:BF:189:THR:O    | 2.51                     | 0.42              |
| 33:BG:119:GLY:C   | 33:BG:181:ARG:HB2  | 2.39                     | 0.42              |
| 36:BN:38:HIS:ND1  | 36:BN:39:ARG:HG3   | 2.34                     | 0.42              |
| 37:BO:78:ARG:CB   | 37:BO:78:ARG:HH11  | 2.16                     | 0.42              |
| 27:BA:389:G:O6    | 38:BP:71:VAL:HB    | 2.19                     | 0.42              |
| 40:BR:61:HIS:O    | 40:BR:65:LEU:HD13  | 2.19                     | 0.42              |
| 27:BA:2873:A:N3   | 40:BR:6:SER:HB2    | 2.34                     | 0.42              |
| 42:BT:108:ARG:HG3 | 42:BT:108:ARG:O    | 2.19                     | 0.42              |
| 31:BE:52:LEU:HD11 | 42:BT:1:MET:CE     | 2.48                     | 0.42              |
| 43:BU:112:ARG:HG2 | 43:BU:112:ARG:HH11 | 1.85                     | 0.42              |
| 43:BU:5:LYS:HB2   | 43:BU:5:LYS:HE3    | 1.84                     | 0.42              |
| 43:BU:76:TYR:O    | 43:BU:80:ILE:HG12  | 2.18                     | 0.42              |
| 46:BX:10:ALA:HA   | 51:B2:37:PHE:CE1   | 2.54                     | 0.42              |
| 27:BA:65:C:P      | 46:BX:71:GLY:HA3   | 2.59                     | 0.42              |
| 48:BZ:104:VAL:O   | 48:BZ:104:VAL:HG22 | 2.19                     | 0.42              |
| 1:CA:102:G:O2'    | 1:CA:103:C:H5'     | 2.19                     | 0.42              |
| 1:CA:1056:U:H4'   | 3:CC:163:ALA:HB2   | 2.01                     | 0.42              |
| 1:CA:1059:C:O2'   | 14:CN:45:ARG:NH2   | 2.52                     | 0.42              |
| 1:CA:1315:U:H2'   | 1:CA:1316:G:C4'    | 2.50                     | 0.42              |
| 1:CA:1372:U:O2'   | 1:CA:1373:G:H5'    | 2.19                     | 0.42              |
| 1:CA:1399:C:O2    | 1:CA:1401:G:C6     | 2.71                     | 0.42              |
| 1:CA:1417:G:H2'   | 1:CA:1482:G:H22    | 1.84                     | 0.42              |
| 1:CA:426:G:H4'    | 4:CD:41:GLY:O      | 2.19                     | 0.42              |
| 1:CA:452:A:H1'    | 16:CP:72:ARG:NH1   | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:662:G:C2     | 1:CA:744:C:C2     | 3.07                     | 0.42              |
| 1:CA:671:G:O2'    | 1:CA:672:U:H5'    | 2.18                     | 0.42              |
| 1:CA:695:A:H2'    | 1:CA:696:A:C8     | 2.54                     | 0.42              |
| 1:CA:737:A:C2     | 1:CA:738:C:C2     | 3.08                     | 0.42              |
| 1:CA:852:G:O2'    | 1:CA:853:G:H5'    | 2.20                     | 0.42              |
| 1:CA:874:G:O2'    | 1:CA:875:C:O5'    | 2.38                     | 0.42              |
| 2:CB:26:PRO:O     | 2:CB:28:PHE:N     | 2.52                     | 0.42              |
| 2:CB:76:GLN:O     | 2:CB:208:ILE:CG1  | 2.67                     | 0.42              |
| 1:CA:1055:A:O2'   | 3:CC:161:GLU:HG3  | 2.19                     | 0.42              |
| 3:CC:34:LEU:HD23  | 3:CC:34:LEU:C     | 2.40                     | 0.42              |
| 5:CE:105:VAL:HB   | 5:CE:106:PRO:HD3  | 1.98                     | 0.42              |
| 6:CF:19:LEU:HG    | 6:CF:19:LEU:O     | 2.19                     | 0.42              |
| 9:CI:5:TYR:HA     | 9:CI:17:VAL:O     | 2.20                     | 0.42              |
| 20:CT:50:GLU:O    | 20:CT:54:LYS:HB2  | 2.19                     | 0.42              |
| 23:CW:18:G:H1'    | 23:CW:19:U:C4     | 2.54                     | 0.42              |
| 25:CY:14:A:H2'    | 25:CY:15:G:O4'    | 2.19                     | 0.42              |
| 51:D2:47:ASN:O    | 51:D2:48:HIS:C    | 2.56                     | 0.42              |
| 51:D2:57:ILE:HA   | 51:D2:57:ILE:HD13 | 1.74                     | 0.42              |
| 55:D6:19:ARG:HH11 | 55:D6:43:CYS:HB2  | 1.85                     | 0.42              |
| 27:DA:130:C:C2'   | 27:DA:131:G:O5'   | 2.67                     | 0.42              |
| 27:DA:1391:U:O2   | 27:DA:1394:U:C4   | 2.71                     | 0.42              |
| 27:DA:1449:A:C6   | 27:DA:1450:G:C4   | 3.07                     | 0.42              |
| 27:DA:1612:C:O3'  | 56:D7:5:TRP:CD1   | 2.66                     | 0.42              |
| 27:DA:1666:G:H2'  | 27:DA:1667:G:O4'  | 2.19                     | 0.42              |
| 27:DA:2122:U:H2'  | 27:DA:2123:G:O4'  | 2.19                     | 0.42              |
| 27:DA:2126:A:N1   | 27:DA:2163:C:C4'  | 2.82                     | 0.42              |
| 27:DA:2335:A:O3'  | 27:DA:2336:A:H8   | 2.01                     | 0.42              |
| 27:DA:2358:G:O2'  | 27:DA:2359:C:H5'  | 2.20                     | 0.42              |
| 27:DA:2403:C:H2'  | 27:DA:2404:C:H6   | 1.83                     | 0.42              |
| 27:DA:2864:G:O2'  | 27:DA:2865:U:H5'  | 2.19                     | 0.42              |
| 27:DA:2873:A:N3   | 40:DR:6:SER:HB3   | 2.34                     | 0.42              |
| 27:DA:753:C:O2'   | 27:DA:754:C:H5'   | 2.19                     | 0.42              |
| 27:DA:754:C:H2'   | 27:DA:755:C:C5    | 2.54                     | 0.42              |
| 27:DA:797:C:O5'   | 27:DA:797:C:H6    | 2.02                     | 0.42              |
| 27:DA:80:G:C2'    | 27:DA:81:G:H5'    | 2.49                     | 0.42              |
| 27:DA:873:G:N2    | 27:DA:905:U:C1'   | 2.77                     | 0.42              |
| 27:DA:957:A:OP1   | 39:DQ:76:LYS:NZ   | 2.43                     | 0.42              |
| 30:DD:148:GLU:C   | 30:DD:189:CYS:SG  | 2.98                     | 0.42              |
| 30:DD:94:LEU:HD23 | 30:DD:95:LEU:H    | 1.83                     | 0.42              |
| 31:DE:167:VAL:O   | 31:DE:168:MET:HG2 | 2.19                     | 0.42              |
| 31:DE:72:VAL:O    | 31:DE:73:GLU:C    | 2.57                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DE:82:ARG:HB3  | 31:DE:83:ASP:H     | 1.55                     | 0.42              |
| 35:DI:133:HIS:ND1 | 35:DI:134:PRO:HD2  | 2.34                     | 0.42              |
| 37:DO:52:VAL:O    | 37:DO:52:VAL:HG13  | 2.19                     | 0.42              |
| 38:DP:107:LYS:C   | 38:DP:109:GLY:N    | 2.72                     | 0.42              |
| 39:DQ:122:GLY:HA2 | 39:DQ:125:LEU:HD12 | 2.01                     | 0.42              |
| 41:DS:49:VAL:CG1  | 41:DS:50:SER:N     | 2.83                     | 0.42              |
| 42:DT:126:ALA:C   | 42:DT:128:GLU:N    | 2.72                     | 0.42              |
| 42:DT:65:LYS:HA   | 42:DT:65:LYS:HZ2   | 1.83                     | 0.42              |
| 44:DV:19:LYS:HG3  | 44:DV:20:LEU:N     | 2.34                     | 0.42              |
| 27:DA:494:G:H4'   | 45:DW:6:ILE:CG2    | 2.49                     | 0.42              |
| 47:DY:74:PRO:O    | 47:DY:80:GLY:HA2   | 2.19                     | 0.42              |
| 48:DZ:47:PHE:O    | 48:DZ:48:ARG:O     | 2.37                     | 0.42              |
| 1:AA:1007:C:H2'   | 1:AA:1008:C:H6     | 1.84                     | 0.42              |
| 1:AA:1030:C:C5    | 1:AA:1032:G:N2     | 2.88                     | 0.42              |
| 1:AA:1138:G:C2    | 1:AA:1140:C:C4     | 3.07                     | 0.42              |
| 1:AA:353:A:H2'    | 1:AA:354:G:OP2     | 2.18                     | 0.42              |
| 1:AA:498:U:O2'    | 1:AA:499:A:H8      | 2.02                     | 0.42              |
| 1:AA:50:A:H1'     | 1:AA:52:G:C8       | 2.54                     | 0.42              |
| 1:AA:555:C:H2'    | 1:AA:556:C:C6      | 2.54                     | 0.42              |
| 2:AB:230:VAL:HB   | 2:AB:231:GLU:H     | 1.66                     | 0.42              |
| 3:AC:132:ARG:O    | 3:AC:136:GLN:CB    | 2.67                     | 0.42              |
| 3:AC:137:ALA:O    | 3:AC:141:VAL:HG23  | 2.20                     | 0.42              |
| 4:AD:110:PHE:CE2  | 4:AD:148:VAL:HG23  | 2.53                     | 0.42              |
| 4:AD:149:ALA:HB3  | 4:AD:152:SER:OG    | 2.18                     | 0.42              |
| 5:AE:110:LEU:O    | 5:AE:111:GLU:C     | 2.58                     | 0.42              |
| 5:AE:67:VAL:HG22  | 5:AE:68:GLU:N      | 2.34                     | 0.42              |
| 6:AF:45:LEU:O     | 6:AF:46:ARG:HG2    | 2.18                     | 0.42              |
| 6:AF:75:LEU:HD23  | 6:AF:76:ALA:N      | 2.34                     | 0.42              |
| 7:AG:120:ILE:HG22 | 7:AG:124:LEU:CD1   | 2.48                     | 0.42              |
| 7:AG:41:ARG:O     | 7:AG:45:ASP:N      | 2.40                     | 0.42              |
| 9:AI:115:GLY:HA2  | 10:AJ:58:ASP:OD1   | 2.19                     | 0.42              |
| 9:AI:5:TYR:CD2    | 9:AI:6:GLY:N       | 2.87                     | 0.42              |
| 11:AK:19:ALA:HA   | 11:AK:32:ILE:HA    | 2.01                     | 0.42              |
| 11:AK:38:ASN:HA   | 11:AK:39:PRO:HD3   | 1.86                     | 0.42              |
| 11:AK:95:ILE:O    | 11:AK:96:ARG:C     | 2.57                     | 0.42              |
| 12:AL:31:ARG:HE   | 12:AL:31:ARG:HB3   | 1.56                     | 0.42              |
| 14:AN:14:PRO:O    | 14:AN:15:LYS:C     | 2.56                     | 0.42              |
| 16:AP:82:GLN:N    | 16:AP:82:GLN:CD    | 2.67                     | 0.42              |
| 18:AR:47:THR:HA   | 18:AR:83:GLU:O     | 2.19                     | 0.42              |
| 1:AA:736:C:C5'    | 18:AR:72:ARG:HE    | 2.32                     | 0.42              |
| 11:AK:107:SER:OG  | 18:AR:86:VAL:CG1   | 2.67                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AX:31:G:C2      | 24:AX:40:C:N3      | 2.87                     | 0.42              |
| 24:AX:52:G:O2'     | 24:AX:53:G:H5'     | 2.20                     | 0.42              |
| 24:AX:63:G:C2      | 24:AX:64:G:C8      | 3.08                     | 0.42              |
| 25:AY:43:C:H2'     | 25:AY:43:C:O2      | 2.20                     | 0.42              |
| 50:B1:63:ALA:C     | 50:B1:65:SER:N     | 2.72                     | 0.42              |
| 27:BA:593:G:O4'    | 57:B8:4:MET:HE3    | 2.19                     | 0.42              |
| 27:BA:1130:U:O2    | 27:BA:2025:C:H5''  | 2.20                     | 0.42              |
| 27:BA:1223:G:C5'   | 27:BA:1224:C:OP2   | 2.67                     | 0.42              |
| 27:BA:1347:G:N3    | 27:BA:1347:G:H2'   | 2.34                     | 0.42              |
| 27:BA:146:G:C5     | 27:BA:147:U:C5     | 3.08                     | 0.42              |
| 27:BA:181:A:C2     | 27:BA:435:C:C5     | 3.05                     | 0.42              |
| 27:BA:181:A:C2     | 27:BA:182:A:N3     | 2.87                     | 0.42              |
| 27:BA:1885:A:H3'   | 27:BA:1886:C:C6    | 2.54                     | 0.42              |
| 27:BA:1899:G:C2    | 27:BA:1903:G:C6    | 3.07                     | 0.42              |
| 27:BA:2144:U:HO2'  | 27:BA:2145:C:H6    | 1.65                     | 0.42              |
| 27:BA:2232:U:O2'   | 27:BA:2233:U:H5'   | 2.20                     | 0.42              |
| 27:BA:2644:G:H2'   | 27:BA:2645:G:O4'   | 2.19                     | 0.42              |
| 27:BA:290:G:O2'    | 27:BA:291:C:H5'    | 2.19                     | 0.42              |
| 27:BA:370:G:O2'    | 27:BA:371:A:OP1    | 2.28                     | 0.42              |
| 27:BA:491:G:O2'    | 27:BA:492:A:C5'    | 2.67                     | 0.42              |
| 27:BA:521:G:H2'    | 27:BA:522:G:H8     | 1.82                     | 0.42              |
| 27:BA:562:U:C2     | 27:BA:572:A:N7     | 2.88                     | 0.42              |
| 27:BA:76:C:H42     | 27:BA:110:G:H1     | 1.67                     | 0.42              |
| 27:BA:817:C:HO2'   | 27:BA:839:U:H5''   | 1.85                     | 0.42              |
| 27:BA:838:C:N3     | 27:BA:839:U:C5     | 2.87                     | 0.42              |
| 28:BB:86:G:O2'     | 28:BB:87:G:H5'     | 2.19                     | 0.42              |
| 29:BC:51:PRO:O     | 29:BC:52:ARG:C     | 2.57                     | 0.42              |
| 30:BD:105:ILE:HD12 | 30:BD:106:ILE:HG23 | 2.02                     | 0.42              |
| 30:BD:105:ILE:HD12 | 30:BD:106:ILE:N    | 2.35                     | 0.42              |
| 30:BD:165:ILE:HG22 | 30:BD:166:GLN:N    | 2.35                     | 0.42              |
| 30:BD:210:GLY:HA2  | 30:BD:213:ARG:CG   | 2.49                     | 0.42              |
| 30:BD:263:ARG:CZ   | 30:BD:263:ARG:HB2  | 2.49                     | 0.42              |
| 31:BE:116:VAL:CG2  | 31:BE:122:PHE:CD2  | 3.01                     | 0.42              |
| 32:BF:4:VAL:HG23   | 32:BF:4:VAL:O      | 2.20                     | 0.42              |
| 32:BF:56:GLU:OE2   | 32:BF:93:LYS:NZ    | 2.42                     | 0.42              |
| 35:BI:102:SER:O    | 35:BI:106:GLY:HA2  | 2.19                     | 0.42              |
| 35:BI:131:LYS:HD2  | 35:BI:132:PRO:HD3  | 2.02                     | 0.42              |
| 36:BN:62:VAL:HG22  | 36:BN:63:THR:H     | 1.84                     | 0.42              |
| 37:BO:103:ALA:O    | 37:BO:105:GLU:N    | 2.52                     | 0.42              |
| 37:BO:31:LYS:HD3   | 37:BO:31:LYS:HA    | 1.91                     | 0.42              |
| 39:BQ:1:MET:SD     | 39:BQ:2:LEU:N      | 2.92                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:BO:80:ASP:OD2  | 42:BT:64:ARG:NH2  | 2.52                     | 0.42              |
| 42:BT:76:PHE:HA   | 42:BT:77:PRO:HD3  | 1.76                     | 0.42              |
| 43:BU:111:GLU:OE2 | 43:BU:111:GLU:HA  | 2.18                     | 0.42              |
| 43:BU:92:ARG:NH2  | 44:BV:11:GLN:HG3  | 2.35                     | 0.42              |
| 45:BW:69:LEU:HD22 | 45:BW:107:LEU:HB3 | 2.01                     | 0.42              |
| 47:BY:39:VAL:O    | 47:BY:40:GLU:CB   | 2.68                     | 0.42              |
| 48:BZ:130:ARG:HG2 | 48:BZ:130:ARG:NH1 | 2.35                     | 0.42              |
| 48:BZ:139:ASP:OD2 | 48:BZ:139:ASP:N   | 2.52                     | 0.42              |
| 48:BZ:116:LEU:HA  | 48:BZ:172:ALA:O   | 2.20                     | 0.42              |
| 1:CA:1028:C:H42   | 1:CA:1034:G:N2    | 2.09                     | 0.42              |
| 1:CA:1126:U:H6    | 1:CA:1126:U:OP1   | 2.02                     | 0.42              |
| 1:CA:1168:A:H2'   | 1:CA:1169:A:C8    | 2.54                     | 0.42              |
| 1:CA:1287:A:C2    | 1:CA:1353:G:H1'   | 2.53                     | 0.42              |
| 1:CA:248:C:O2     | 1:CA:248:C:H2'    | 2.20                     | 0.42              |
| 1:CA:324:G:OP1    | 20:CT:70:SER:HB2  | 2.19                     | 0.42              |
| 1:CA:507:C:O5'    | 1:CA:508:C:H3'    | 2.19                     | 0.42              |
| 1:CA:563:A:O2'    | 1:CA:567:G:C8     | 2.71                     | 0.42              |
| 1:CA:811:C:C5     | 1:CA:812:C:C4     | 3.08                     | 0.42              |
| 3:CC:151:VAL:HG12 | 3:CC:152:ILE:N    | 2.34                     | 0.42              |
| 8:CH:6:ILE:HG22   | 8:CH:10:LEU:HD12  | 2.00                     | 0.42              |
| 9:CI:27:THR:O     | 9:CI:63:ILE:HB    | 2.20                     | 0.42              |
| 9:CI:69:GLY:O     | 9:CI:73:GLN:HG3   | 2.19                     | 0.42              |
| 9:CI:79:LEU:CD2   | 9:CI:102:LEU:HD22 | 2.49                     | 0.42              |
| 10:CJ:47:PHE:CZ   | 14:CN:37:PHE:HE2  | 2.37                     | 0.42              |
| 11:CK:123:LYS:HA  | 11:CK:126:ARG:CG  | 2.47                     | 0.42              |
| 11:CK:15:ALA:HB1  | 11:CK:78:GLN:HG3  | 2.01                     | 0.42              |
| 11:CK:53:SER:O    | 11:CK:55:LYS:N    | 2.52                     | 0.42              |
| 12:CL:71:GLY:O    | 12:CL:72:HIS:HB3  | 2.19                     | 0.42              |
| 50:D1:72:GLU:OE1  | 50:D1:76:ARG:HD3  | 2.20                     | 0.42              |
| 51:D2:30:ARG:O    | 51:D2:33:MET:N    | 2.53                     | 0.42              |
| 55:D6:48:VAL:CG2  | 55:D6:49:HIS:N    | 2.82                     | 0.42              |
| 57:D8:21:LYS:HD3  | 57:D8:48:PHE:CE1  | 2.54                     | 0.42              |
| 27:DA:1167:U:H2'  | 27:DA:1168:G:C8   | 2.55                     | 0.42              |
| 27:DA:1478:G:OP1  | 27:DA:1478:G:H4'  | 2.18                     | 0.42              |
| 27:DA:1629:U:H2'  | 27:DA:1630:G:C8   | 2.54                     | 0.42              |
| 27:DA:1973:G:H2'  | 27:DA:1974:C:C5   | 2.53                     | 0.42              |
| 27:DA:229:A:H3'   | 27:DA:229:A:C8    | 2.55                     | 0.42              |
| 27:DA:2366:A:C6   | 27:DA:2367:G:C4   | 3.07                     | 0.42              |
| 27:DA:2510:C:O2   | 27:DA:2510:C:H2'  | 2.18                     | 0.42              |
| 27:DA:2544:G:N3   | 27:DA:2545:G:C8   | 2.88                     | 0.42              |
| 27:DA:2792:G:O2'  | 27:DA:2793:G:C8   | 2.69                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:2805:G:C2   | 27:DA:2807:G:C4    | 3.08                     | 0.42              |
| 27:DA:408:G:O2'   | 27:DA:409:C:H5'    | 2.20                     | 0.42              |
| 27:DA:632:A:O2'   | 27:DA:633:A:H5'    | 2.20                     | 0.42              |
| 27:DA:849:A:OP2   | 27:DA:850:C:H5     | 2.01                     | 0.42              |
| 28:DB:11:C:P      | 28:DB:12:C:H5      | 2.43                     | 0.42              |
| 29:DC:51:PRO:HG3  | 29:DC:204:ALA:CB   | 2.42                     | 0.42              |
| 27:DA:1792:G:H5'' | 30:DD:205:VAL:HG13 | 2.00                     | 0.42              |
| 27:DA:2052:G:N2   | 31:DE:149:ARG:HA   | 2.17                     | 0.42              |
| 27:DA:2733:A:C2   | 31:DE:203:LYS:HA   | 2.51                     | 0.42              |
| 32:DF:152:GLU:O   | 32:DF:154:VAL:HG23 | 2.18                     | 0.42              |
| 35:DI:120:ILE:O   | 35:DI:121:LYS:HB3  | 2.20                     | 0.42              |
| 36:DN:132:ALA:O   | 36:DN:133:GLN:CB   | 2.66                     | 0.42              |
| 37:DO:53:LYS:N    | 37:DO:53:LYS:CD    | 2.80                     | 0.42              |
| 38:DP:13:ASN:ND2  | 38:DP:14:LYS:HG3   | 2.34                     | 0.42              |
| 38:DP:75:ILE:CG2  | 38:DP:76:LYS:N     | 2.81                     | 0.42              |
| 38:DP:88:LEU:C    | 38:DP:90:ARG:H     | 2.21                     | 0.42              |
| 39:DQ:52:VAL:O    | 39:DQ:55:VAL:HG12  | 2.20                     | 0.42              |
| 40:DR:51:LEU:O    | 40:DR:54:LEU:HB2   | 2.20                     | 0.42              |
| 40:DR:93:GLY:C    | 40:DR:95:THR:N     | 2.73                     | 0.42              |
| 43:DU:105:VAL:O   | 43:DU:108:GLU:HB2  | 2.19                     | 0.42              |
| 43:DU:33:ARG:O    | 43:DU:35:ALA:N     | 2.52                     | 0.42              |
| 43:DU:92:ARG:O    | 43:DU:94:ASN:N     | 2.50                     | 0.42              |
| 44:DV:59:ALA:CB   | 44:DV:96:ILE:HA    | 2.44                     | 0.42              |
| 47:DY:27:VAL:CG1  | 47:DY:29:GLU:OE1   | 2.67                     | 0.42              |
| 47:DY:31:LEU:CB   | 47:DY:32:PRO:HA    | 2.49                     | 0.42              |
| 48:DZ:107:PRO:CG  | 48:DZ:116:LEU:HB2  | 2.50                     | 0.42              |
| 48:DZ:88:PHE:O    | 48:DZ:90:LEU:CD1   | 2.68                     | 0.42              |
| 1:AA:110:C:H2'    | 1:AA:111:G:H5'     | 2.02                     | 0.42              |
| 1:AA:1333:A:C2'   | 1:AA:1334:G:O5'    | 2.67                     | 0.42              |
| 1:AA:1498:U:H5''  | 1:AA:1499:A:OP1    | 2.19                     | 0.42              |
| 1:AA:158:G:C6     | 1:AA:159:G:N7      | 2.88                     | 0.42              |
| 1:AA:38:G:H4'     | 1:AA:547:A:C6      | 2.55                     | 0.42              |
| 1:AA:56:U:O2'     | 1:AA:57:G:H5'      | 2.20                     | 0.42              |
| 1:AA:690:G:C6     | 1:AA:691:G:C6      | 3.07                     | 0.42              |
| 1:AA:758:G:H2'    | 1:AA:759:A:OP2     | 2.20                     | 0.42              |
| 1:AA:818:G:HO2'   | 1:AA:820:U:H6      | 1.64                     | 0.42              |
| 1:AA:840:C:C4'    | 1:AA:841:U:OP1     | 2.68                     | 0.42              |
| 2:AB:32:ILE:CG1   | 2:AB:33:TYR:N      | 2.81                     | 0.42              |
| 3:AC:14:ILE:HG12  | 3:AC:15:THR:N      | 2.35                     | 0.42              |
| 5:AE:132:ALA:C    | 5:AE:134:ALA:H     | 2.23                     | 0.42              |
| 5:AE:26:PHE:HD1   | 5:AE:26:PHE:H      | 1.67                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:53:LEU:N      | 5:AE:53:LEU:CD1    | 2.83                     | 0.42              |
| 8:AH:87:SER:HA     | 8:AH:93:VAL:HG23   | 2.01                     | 0.42              |
| 10:AJ:30:SER:CB    | 10:AJ:81:THR:HG23  | 2.49                     | 0.42              |
| 1:AA:1124:G:H5'    | 10:AJ:35:SER:HB2   | 2.01                     | 0.42              |
| 12:AL:31:ARG:O     | 12:AL:57:LEU:HD12  | 2.19                     | 0.42              |
| 1:AA:740:U:H4'     | 15:AO:39:LEU:HD23  | 2.02                     | 0.42              |
| 16:AP:68:ASP:C     | 16:AP:70:ALA:N     | 2.73                     | 0.42              |
| 23:AW:12:C:OP2     | 23:AW:12:C:H6      | 2.03                     | 0.42              |
| 23:AW:7:A:O2'      | 23:AW:8:U:P        | 2.77                     | 0.42              |
| 25:AY:34:U:O2'     | 25:AY:35:G:H5'     | 2.20                     | 0.42              |
| 50:B1:46:LEU:N     | 50:B1:46:LEU:CD2   | 2.82                     | 0.42              |
| 51:B2:21:LEU:CD1   | 51:B2:64:LEU:HA    | 2.48                     | 0.42              |
| 52:B3:11:SER:HA    | 52:B3:31:LEU:HD21  | 2.01                     | 0.42              |
| 55:B6:15:GLU:CD    | 55:B6:18:ARG:HG3   | 2.40                     | 0.42              |
| 27:BA:106:C:O5'    | 27:BA:106:C:H6     | 2.02                     | 0.42              |
| 27:BA:1238:G:H2'   | 27:BA:1239:G:O4'   | 2.20                     | 0.42              |
| 27:BA:1421:G:C2    | 27:BA:1422:G:C8    | 3.08                     | 0.42              |
| 27:BA:1603:A:H3'   | 27:BA:1604:C:C6    | 2.54                     | 0.42              |
| 27:BA:1673:U:C2'   | 27:BA:1674:G:H5''  | 2.47                     | 0.42              |
| 27:BA:18:C:H2'     | 27:BA:19:C:C6      | 2.54                     | 0.42              |
| 27:BA:2070:G:C2    | 27:BA:2071:A:N3    | 2.87                     | 0.42              |
| 27:BA:2420:C:OP1   | 57:B8:34:TRP:HB2   | 2.20                     | 0.42              |
| 27:BA:251:A:H2'    | 27:BA:252:G:C4'    | 2.49                     | 0.42              |
| 27:BA:2562:U:H2'   | 27:BA:2563:U:C5'   | 2.47                     | 0.42              |
| 27:BA:355:G:C5     | 27:BA:356:G:N7     | 2.88                     | 0.42              |
| 27:BA:463:G:C2     | 27:BA:467:G:C6     | 3.08                     | 0.42              |
| 27:BA:479:A:H4'    | 27:BA:480:A:H5'    | 2.01                     | 0.42              |
| 27:BA:49:A:N6      | 27:BA:118:A:C8     | 2.87                     | 0.42              |
| 27:BA:500:G:N2     | 27:BA:502:A:H3'    | 2.34                     | 0.42              |
| 27:BA:866:A:C8     | 27:BA:866:A:O5'    | 2.73                     | 0.42              |
| 29:BC:49:ILE:O     | 29:BC:51:PRO:N     | 2.52                     | 0.42              |
| 30:BD:166:GLN:HB3  | 30:BD:174:ILE:CG2  | 2.48                     | 0.42              |
| 30:BD:31:LYS:CE    | 30:BD:33:LEU:HD22  | 2.33                     | 0.42              |
| 30:BD:43:ARG:HB2   | 30:BD:54:ARG:HB2   | 2.02                     | 0.42              |
| 31:BE:175:VAL:HG12 | 31:BE:182:LEU:HD12 | 2.01                     | 0.42              |
| 32:BF:66:PRO:HD2   | 32:BF:70:THR:CG2   | 2.32                     | 0.42              |
| 33:BG:95:ARG:O     | 33:BG:96:ARG:O     | 2.37                     | 0.42              |
| 35:BI:68:LEU:HA    | 35:BI:71:ILE:CD1   | 2.50                     | 0.42              |
| 37:BO:114:ILE:O    | 37:BO:115:VAL:C    | 2.57                     | 0.42              |
| 38:BP:18:ARG:HB3   | 38:BP:18:ARG:NH1   | 2.34                     | 0.42              |
| 41:BS:14:VAL:CG1   | 41:BS:15:ARG:H     | 2.25                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BT:89:VAL:HG11 | 42:BT:91:ARG:NE    | 2.35                     | 0.42              |
| 47:BY:60:PHE:CA   | 47:BY:62:GLU:OE2   | 2.67                     | 0.42              |
| 39:BQ:63:LYS:NZ   | 48:BZ:174:VAL:HG21 | 2.34                     | 0.42              |
| 1:CA:1069:C:H42   | 1:CA:1106:G:H1     | 1.67                     | 0.42              |
| 1:CA:1303:C:H2'   | 1:CA:1304:G:O4'    | 2.19                     | 0.42              |
| 1:CA:135:C:C2'    | 1:CA:136:C:H5'     | 2.46                     | 0.42              |
| 1:CA:252:U:C2     | 1:CA:253:U:H5      | 2.37                     | 0.42              |
| 1:CA:373:A:N3     | 1:CA:374:A:C8      | 2.88                     | 0.42              |
| 1:CA:383:A:H2'    | 1:CA:384:G:C5'     | 2.49                     | 0.42              |
| 1:CA:486:U:H2'    | 1:CA:487:A:C8      | 2.54                     | 0.42              |
| 1:CA:507:C:C2'    | 1:CA:508:C:C5      | 3.00                     | 0.42              |
| 1:CA:898:G:N2     | 1:CA:901:A:C8      | 2.87                     | 0.42              |
| 1:CA:922:G:C5     | 1:CA:923:A:C5      | 3.07                     | 0.42              |
| 2:CB:228:GLY:O    | 2:CB:230:VAL:HG13  | 2.19                     | 0.42              |
| 1:CA:1111:A:N1    | 3:CC:177:THR:HG23  | 2.35                     | 0.42              |
| 1:CA:1206:G:C4'   | 3:CC:192:THR:O     | 2.64                     | 0.42              |
| 4:CD:77:ASN:O     | 4:CD:78:LEU:C      | 2.56                     | 0.42              |
| 5:CE:8:GLU:OE2    | 5:CE:63:ARG:NH2    | 2.53                     | 0.42              |
| 7:CG:108:ALA:C    | 7:CG:110:GLN:H     | 2.22                     | 0.42              |
| 7:CG:103:TRP:HB3  | 7:CG:134:ALA:HB1   | 2.01                     | 0.42              |
| 7:CG:15:ASP:CG    | 7:CG:44:TYR:HH     | 2.22                     | 0.42              |
| 7:CG:75:VAL:HA    | 7:CG:88:PRO:HA     | 2.01                     | 0.42              |
| 7:CG:80:VAL:HG11  | 7:CG:154:TYR:CZ    | 2.54                     | 0.42              |
| 10:CJ:51:ARG:HG3  | 10:CJ:60:ARG:HA    | 2.01                     | 0.42              |
| 10:CJ:63:PHE:CD2  | 10:CJ:63:PHE:N     | 2.88                     | 0.42              |
| 10:CJ:4:ILE:CG1   | 10:CJ:77:PRO:HG3   | 2.50                     | 0.42              |
| 17:CQ:27:PHE:N    | 17:CQ:27:PHE:HD2   | 2.17                     | 0.42              |
| 20:CT:30:LYS:O    | 20:CT:31:SER:C     | 2.57                     | 0.42              |
| 51:D2:31:GLU:O    | 51:D2:32:LEU:C     | 2.58                     | 0.42              |
| 55:D6:22:ALA:O    | 55:D6:23:THR:CB    | 2.67                     | 0.42              |
| 55:D6:27:LYS:HB3  | 55:D6:29:ASN:OD1   | 2.20                     | 0.42              |
| 27:DA:81:G:C2     | 27:DA:106:C:N3     | 2.88                     | 0.42              |
| 27:DA:1210:A:C6   | 27:DA:1237:A:N7    | 2.88                     | 0.42              |
| 27:DA:1695:G:C2'  | 27:DA:1695:G:N3    | 2.80                     | 0.42              |
| 27:DA:1777:U:C2'  | 27:DA:1778:U:O5'   | 2.67                     | 0.42              |
| 27:DA:1796:U:O2'  | 27:DA:1797:C:H5'   | 2.20                     | 0.42              |
| 27:DA:182:A:N3    | 27:DA:433:C:O2'    | 2.43                     | 0.42              |
| 27:DA:2069:G:C2'  | 27:DA:2070:G:H5'   | 2.49                     | 0.42              |
| 27:DA:2463:C:O2   | 27:DA:2488:A:C2    | 2.73                     | 0.42              |
| 27:DA:2681:C:H5   | 27:DA:2725:A:N6    | 2.06                     | 0.42              |
| 27:DA:2683:C:O2'  | 27:DA:2684:U:H5'   | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:272(B):G:O2' | 27:DA:272(C):G:P   | 2.78                     | 0.42              |
| 27:DA:2808:U:HO2'  | 27:DA:2809:A:H5'   | 1.78                     | 0.42              |
| 27:DA:2824:C:C4    | 27:DA:2825:C:C2    | 3.08                     | 0.42              |
| 27:DA:220:G:N2     | 27:DA:427:U:H2'    | 2.34                     | 0.42              |
| 27:DA:638:G:H2'    | 27:DA:639:U:O4'    | 2.20                     | 0.42              |
| 27:DA:669:G:H2'    | 27:DA:669:G:N3     | 2.35                     | 0.42              |
| 27:DA:682:G:N2     | 27:DA:796:C:C2     | 2.88                     | 0.42              |
| 27:DA:845:G:C8     | 27:DA:845:G:OP2    | 2.72                     | 0.42              |
| 27:DA:868:U:H2'    | 27:DA:869:G:O4'    | 2.20                     | 0.42              |
| 27:DA:907:U:H6     | 27:DA:907:U:C5'    | 2.33                     | 0.42              |
| 27:DA:942:G:H5''   | 38:DP:36:LYS:O     | 2.19                     | 0.42              |
| 27:DA:94:C:O2      | 27:DA:94:C:H2'     | 2.18                     | 0.42              |
| 29:DC:128:GLY:C    | 29:DC:130:ILE:H    | 2.22                     | 0.42              |
| 29:DC:51:PRO:HB3   | 29:DC:203:GLY:C    | 2.39                     | 0.42              |
| 29:DC:64:LEU:C     | 29:DC:66:HIS:H     | 2.23                     | 0.42              |
| 30:DD:134:ARG:HG3  | 30:DD:135:PHE:CD2  | 2.55                     | 0.42              |
| 27:DA:691:C:H1'    | 30:DD:43:ARG:CZ    | 2.50                     | 0.42              |
| 31:DE:54:GLN:HB2   | 31:DE:55:ASN:H     | 1.48                     | 0.42              |
| 32:DF:101:LEU:O    | 32:DF:106:ARG:NH1  | 2.50                     | 0.42              |
| 34:DH:20:ALA:HB1   | 34:DH:21:PRO:HD2   | 2.02                     | 0.42              |
| 35:DI:97:ILE:O     | 35:DI:97:ILE:HG22  | 2.19                     | 0.42              |
| 36:DN:57:ALA:C     | 36:DN:58:ASP:OD1   | 2.57                     | 0.42              |
| 37:DO:43:VAL:O     | 37:DO:54:GLU:HA    | 2.20                     | 0.42              |
| 37:DO:67:LYS:O     | 37:DO:68:GLU:C     | 2.57                     | 0.42              |
| 38:DP:9:ASN:H      | 38:DP:10:PRO:HD3   | 1.84                     | 0.42              |
| 39:DQ:38:GLU:CG    | 39:DQ:127:ILE:HG22 | 2.46                     | 0.42              |
| 39:DQ:132:VAL:CG1  | 48:DZ:80:ARG:NH2   | 2.83                     | 0.42              |
| 39:DQ:3:MET:HB2    | 39:DQ:93:TYR:CE1   | 2.54                     | 0.42              |
| 39:DQ:85:LYS:HG3   | 49:D0:7:LEU:HB3    | 2.01                     | 0.42              |
| 40:DR:28:LEU:HD21  | 40:DR:114:VAL:HG12 | 2.01                     | 0.42              |
| 42:DT:35:LYS:CE    | 42:DT:41:ARG:HE    | 2.32                     | 0.42              |
| 44:DV:12:TYR:O     | 44:DV:14:VAL:HG13  | 2.19                     | 0.42              |
| 45:DW:29:LEU:HD23  | 45:DW:69:LEU:HD12  | 2.01                     | 0.42              |
| 47:DY:32:PRO:O     | 47:DY:35:TYR:N     | 2.53                     | 0.42              |
| 1:AA:1084:G:C5     | 1:AA:1085:U:C4     | 3.07                     | 0.42              |
| 1:AA:108:G:O6      | 20:AT:15:ARG:HD2   | 2.20                     | 0.42              |
| 1:AA:1123:A:O3'    | 10:AJ:36:GLY:HA3   | 2.19                     | 0.42              |
| 1:AA:113:G:O2'     | 1:AA:114:U:P       | 2.78                     | 0.42              |
| 1:AA:1278:U:H5'    | 1:AA:1279:A:C4     | 2.55                     | 0.42              |
| 1:AA:1340:A:C2     | 1:AA:1341:U:O2     | 2.73                     | 0.42              |
| 1:AA:1401:G:H2'    | 1:AA:1402:C:O4'    | 2.20                     | 0.42              |

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| Atom-1               | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-------------------|--------------------------|-------------------|
| 1:AA:1504:G:OP1      | 1:AA:1507:A:H4'   | 2.20                     | 0.42              |
| 1:AA:684:A:C6        | 1:AA:685:G:C6     | 3.07                     | 0.42              |
| 1:AA:687:A:O2'       | 1:AA:688:G:OP2    | 2.31                     | 0.42              |
| 1:AA:859:A:H2'       | 1:AA:860:A:O4'    | 2.18                     | 0.42              |
| 1:AA:913:A:O2'       | 1:AA:914:A:OP2    | 2.24                     | 0.42              |
| 3:AC:134:ILE:HD12    | 3:AC:151:VAL:CG1  | 2.49                     | 0.42              |
| 3:AC:130:VAL:O       | 3:AC:134:ILE:HG12 | 2.20                     | 0.42              |
| 5:AE:149:GLU:C       | 5:AE:151:LEU:N    | 2.73                     | 0.42              |
| 5:AE:76:ILE:CG1      | 5:AE:77:PRO:CD    | 2.95                     | 0.42              |
| 6:AF:17:SER:O        | 6:AF:21:LEU:HD23  | 2.19                     | 0.42              |
| 7:AG:151:TYR:CD1     | 7:AG:151:TYR:N    | 2.87                     | 0.42              |
| 7:AG:51:GLN:O        | 7:AG:54:THR:O     | 2.36                     | 0.42              |
| 7:AG:95:ARG:HG3      | 7:AG:95:ARG:HH11  | 1.85                     | 0.42              |
| 10:AJ:22:LYS:HZ2     | 10:AJ:23:ILE:HG12 | 1.85                     | 0.42              |
| 10:AJ:42:THR:HG23    | 10:AJ:68:HIS:HA   | 2.00                     | 0.42              |
| 11:AK:126:ARG:HB3    | 11:AK:126:ARG:CZ  | 2.50                     | 0.42              |
| 12:AL:25:LYS:HG3     | 12:AL:30:ARG:HH12 | 1.85                     | 0.42              |
| 1:AA:520:A:OP2       | 12:AL:48:ALA:HB1  | 2.19                     | 0.42              |
| 14:AN:19:ARG:O       | 14:AN:21:TYR:CD1  | 2.72                     | 0.42              |
| 15:AO:41:GLU:C       | 15:AO:43:LEU:N    | 2.72                     | 0.42              |
| 20:AT:35:THR:O       | 20:AT:38:LYS:HB2  | 2.20                     | 0.42              |
| 20:AT:57:ARG:HH11    | 20:AT:57:ARG:HB2  | 1.84                     | 0.42              |
| 51:B2:41:ILE:O       | 51:B2:42:GLY:C    | 2.58                     | 0.42              |
| 51:B2:53:LEU:HA      | 51:B2:53:LEU:HD23 | 1.83                     | 0.42              |
| 54:B5:51:TYR:HB3     | 54:B5:52:TYR:H    | 1.44                     | 0.42              |
| 57:B8:2:PRO:O        | 57:B8:3:LYS:C     | 2.58                     | 0.42              |
| 27:BA:1146:C:C4      | 27:BA:1147:C:C5   | 3.08                     | 0.42              |
| 27:BA:1303:G:C2      | 27:BA:1304:C:C5   | 3.07                     | 0.42              |
| 27:BA:1649:G:O2'     | 27:BA:1650:G:H5'  | 2.20                     | 0.42              |
| 27:BA:1745(A):C:H5'' | 27:BA:1746:G:OP2  | 2.19                     | 0.42              |
| 27:BA:1922:G:H2'     | 27:BA:1923:U:H6   | 1.84                     | 0.42              |
| 27:BA:2080:G:C4      | 27:BA:2081:C:C5   | 3.07                     | 0.42              |
| 27:BA:2082:A:H2'     | 27:BA:2083:G:C8   | 2.54                     | 0.42              |
| 27:BA:227:A:H5'      | 27:BA:228:A:C2    | 2.55                     | 0.42              |
| 27:BA:2386:C:H2'     | 27:BA:2387:U:H6   | 1.82                     | 0.42              |
| 27:BA:2424:C:O2'     | 27:BA:2425:A:OP1  | 2.37                     | 0.42              |
| 27:BA:2436:G:C6      | 27:BA:2437:U:C4   | 3.07                     | 0.42              |
| 27:BA:2518:A:H8      | 27:BA:2518:A:H5'  | 1.85                     | 0.42              |
| 27:BA:2568:C:H2'     | 27:BA:2569:G:O4'  | 2.19                     | 0.42              |
| 27:BA:2654:A:OP1     | 27:BA:2654:A:H8   | 2.02                     | 0.42              |
| 27:BA:40:C:H2'       | 27:BA:41:C:C6     | 2.43                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:451:C:C4    | 27:BA:453:C:C6     | 3.08                     | 0.42              |
| 27:BA:699:A:C2'   | 27:BA:700:G:H5'    | 2.50                     | 0.42              |
| 27:BA:843:G:C2    | 27:BA:936:C:N3     | 2.87                     | 0.42              |
| 27:BA:94:C:H5'    | 27:BA:94(A):G:OP2  | 2.20                     | 0.42              |
| 27:BA:959:A:C6    | 27:BA:960:A:C6     | 3.08                     | 0.42              |
| 27:BA:950:G:C2    | 27:BA:968:G:N3     | 2.88                     | 0.42              |
| 28:BB:43:C:H5'    | 28:BB:44:G:OP2     | 2.19                     | 0.42              |
| 29:BC:121:GLY:CA  | 29:BC:145:VAL:HA   | 2.48                     | 0.42              |
| 29:BC:155:GLU:O   | 29:BC:156:ILE:CB   | 2.67                     | 0.42              |
| 29:BC:47:LEU:HB3  | 29:BC:207:THR:HA   | 2.02                     | 0.42              |
| 29:BC:98:GLU:C    | 29:BC:100:ILE:H    | 2.21                     | 0.42              |
| 30:BD:123:ALA:HB3 | 30:BD:131:LEU:HG   | 2.02                     | 0.42              |
| 31:BE:143:ASN:OD1 | 31:BE:147:PRO:CD   | 2.67                     | 0.42              |
| 32:BF:124:LEU:O   | 32:BF:125:LEU:HD12 | 2.19                     | 0.42              |
| 33:BG:29:TRP:HA   | 33:BG:33:ARG:NH1   | 2.34                     | 0.42              |
| 33:BG:96:ARG:O    | 33:BG:97:ASP:C     | 2.57                     | 0.42              |
| 34:BH:150:ALA:C   | 34:BH:152:ARG:H    | 2.23                     | 0.42              |
| 35:BI:79:ILE:HG12 | 35:BI:140:LEU:HD11 | 2.01                     | 0.42              |
| 39:BQ:42:ILE:N    | 39:BQ:42:ILE:HD12  | 2.34                     | 0.42              |
| 27:BA:2483:C:C2'  | 39:BQ:49:ALA:HB1   | 2.49                     | 0.42              |
| 40:BR:62:ALA:O    | 40:BR:65:LEU:HB2   | 2.20                     | 0.42              |
| 41:BS:67:ARG:HG2  | 41:BS:67:ARG:NH1   | 2.35                     | 0.42              |
| 42:BT:29:ARG:HH21 | 42:BT:88:ILE:HD11  | 1.85                     | 0.42              |
| 44:BV:10:LYS:HD2  | 44:BV:12:TYR:OH    | 2.19                     | 0.42              |
| 45:BW:64:MET:HB3  | 45:BW:109:GLU:CD   | 2.39                     | 0.42              |
| 45:BW:18:ARG:HG2  | 45:BW:18:ARG:HH11  | 1.85                     | 0.42              |
| 48:BZ:124:LEU:HG  | 48:BZ:163:ALA:CB   | 2.50                     | 0.42              |
| 1:CA:1045:C:H2'   | 1:CA:1045:C:O2     | 2.19                     | 0.42              |
| 1:CA:1060:C:H4'   | 10:CJ:52:GLY:N     | 2.35                     | 0.42              |
| 1:CA:119:A:H5''   | 1:CA:120:A:C5'     | 2.47                     | 0.42              |
| 1:CA:1218:C:H2'   | 1:CA:1219:U:C6     | 2.54                     | 0.42              |
| 1:CA:1427:U:H2'   | 1:CA:1428:A:H8     | 1.79                     | 0.42              |
| 1:CA:189(F):U:H5  | 17:CQ:3:LYS:NZ     | 2.17                     | 0.42              |
| 1:CA:227:G:C4     | 1:CA:228:A:C8      | 3.08                     | 0.42              |
| 1:CA:431:A:H2'    | 1:CA:432:A:C8      | 2.55                     | 0.42              |
| 1:CA:53:A:C6      | 1:CA:54:C:C2       | 3.08                     | 0.42              |
| 1:CA:650:G:O2'    | 1:CA:651:C:H5'     | 2.20                     | 0.42              |
| 1:CA:652:U:C5     | 1:CA:752:G:C5      | 3.08                     | 0.42              |
| 1:CA:749:C:O2'    | 1:CA:750:G:C5'     | 2.66                     | 0.42              |
| 1:CA:768:A:H8     | 1:CA:768:A:O5'     | 2.02                     | 0.42              |
| 1:CA:979:C:C2'    | 1:CA:980:C:H5''    | 2.49                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CC:20:SER:OG    | 3:CC:57:ILE:HB     | 2.20                     | 0.42              |
| 4:CD:178:VAL:O    | 4:CD:179:GLU:C     | 2.57                     | 0.42              |
| 5:CE:107:ARG:CG   | 5:CE:108:ALA:N     | 2.82                     | 0.42              |
| 7:CG:137:LYS:O    | 7:CG:138:LYS:C     | 2.58                     | 0.42              |
| 7:CG:6:ARG:HG2    | 7:CG:6:ARG:O       | 2.18                     | 0.42              |
| 8:CH:75:ARG:HA    | 8:CH:76:PRO:HD2    | 1.80                     | 0.42              |
| 9:CI:27:THR:CG2   | 9:CI:31:GLN:N      | 2.82                     | 0.42              |
| 15:CO:9:GLN:HB3   | 15:CO:13:GLN:NE2   | 2.34                     | 0.42              |
| 24:CX:34:C:O2     | 24:CX:34:C:C2'     | 2.62                     | 0.42              |
| 52:D3:39:ASP:OD2  | 52:D3:44:ARG:NE    | 2.53                     | 0.42              |
| 56:D7:27:GLY:O    | 56:D7:28:ARG:C     | 2.58                     | 0.42              |
| 57:D8:33:ASN:HA   | 57:D8:36:LYS:CD    | 2.50                     | 0.42              |
| 27:DA:1484:G:N1   | 27:DA:1506:C:C2    | 2.88                     | 0.42              |
| 27:DA:154:G:C6    | 27:DA:154(A):C:C4  | 3.08                     | 0.42              |
| 27:DA:1649:G:C6   | 27:DA:2009:G:C6    | 3.08                     | 0.42              |
| 27:DA:171:G:C5    | 27:DA:172:C:N4     | 2.88                     | 0.42              |
| 27:DA:1831:G:C5   | 27:DA:1975:G:C2    | 3.08                     | 0.42              |
| 27:DA:2110:G:C6   | 27:DA:2120:G:N7    | 2.87                     | 0.42              |
| 27:DA:185:U:H4'   | 27:DA:218:A:H4'    | 2.01                     | 0.42              |
| 27:DA:2347:C:H6   | 27:DA:2347:C:H5''  | 1.85                     | 0.42              |
| 27:DA:234:C:H6    | 27:DA:234:C:O5'    | 2.02                     | 0.42              |
| 27:DA:2291:U:O2'  | 27:DA:2374:C:H1'   | 2.20                     | 0.42              |
| 27:DA:2448:A:O2'  | 27:DA:2449:U:H5    | 2.02                     | 0.42              |
| 27:DA:2450:A:H2'  | 27:DA:2451:A:H8    | 1.84                     | 0.42              |
| 27:DA:2520:C:C2   | 27:DA:2521:C:C6    | 3.08                     | 0.42              |
| 27:DA:2645:G:H4'  | 27:DA:2646:C:OP2   | 2.19                     | 0.42              |
| 27:DA:2693:A:H2'  | 27:DA:2694:G:C8    | 2.55                     | 0.42              |
| 27:DA:469:G:O6    | 56:D7:37:LYS:NZ    | 2.40                     | 0.42              |
| 27:DA:592:G:H21   | 57:D8:4:MET:HE1    | 1.84                     | 0.42              |
| 27:DA:660:G:N1    | 27:DA:661:C:C2     | 2.87                     | 0.42              |
| 27:DA:864:G:O5'   | 27:DA:864:G:H8     | 2.03                     | 0.42              |
| 27:DA:872:A:C2    | 27:DA:906:G:C4     | 3.08                     | 0.42              |
| 27:DA:858:U:N3    | 27:DA:920:G:N2     | 2.67                     | 0.42              |
| 30:DD:254:THR:OG1 | 30:DD:254:THR:O    | 2.37                     | 0.42              |
| 30:DD:33:LEU:CD1  | 30:DD:33:LEU:H     | 2.32                     | 0.42              |
| 33:DG:128:ARG:HB2 | 33:DG:130:ASN:O    | 2.20                     | 0.42              |
| 33:DG:42:GLY:O    | 33:DG:88:ILE:HG13  | 2.20                     | 0.42              |
| 33:DG:5:VAL:C     | 33:DG:7:LEU:H      | 2.23                     | 0.42              |
| 33:DG:81:LYS:O    | 33:DG:82:LEU:C     | 2.57                     | 0.42              |
| 35:DI:83:ALA:HA   | 35:DI:89:TYR:HD1   | 1.82                     | 0.42              |
| 37:DO:104:ARG:NH1 | 37:DO:121:VAL:HG12 | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:DU:102:GLU:HA  | 43:DU:103:PRO:HD2 | 1.88                     | 0.42              |
| 27:DA:995:C:H5''  | 43:DU:54:LYS:HE3  | 2.02                     | 0.42              |
| 45:DW:100:THR:OG1 | 45:DW:101:SER:N   | 2.52                     | 0.42              |
| 45:DW:90:ARG:NH1  | 45:DW:90:ARG:HG3  | 2.35                     | 0.42              |
| 47:DY:2:ARG:O     | 47:DY:3:VAL:CG2   | 2.68                     | 0.42              |
| 48:DZ:132:ILE:HA  | 48:DZ:133:PRO:HD2 | 1.75                     | 0.42              |
| 1:AA:988:G:H21    | 1:AA:1015:A:H2    | 1.68                     | 0.42              |
| 1:AA:1138:G:H2'   | 1:AA:1140:C:C6    | 2.55                     | 0.42              |
| 1:AA:1152:A:O2'   | 1:AA:1153:C:OP2   | 2.36                     | 0.42              |
| 1:AA:1183:A:H3'   | 1:AA:1184:G:C5'   | 2.49                     | 0.42              |
| 1:AA:1065:U:C4    | 1:AA:1190:G:H1'   | 2.55                     | 0.42              |
| 1:AA:1242:C:O2'   | 1:AA:1243:C:H5'   | 2.19                     | 0.42              |
| 1:AA:1285:A:O4'   | 1:AA:1286:A:C8    | 2.71                     | 0.42              |
| 1:AA:129(A):G:C2  | 1:AA:189(H):G:N7  | 2.88                     | 0.42              |
| 1:AA:253:U:H5'    | 1:AA:253:U:C6     | 2.50                     | 0.42              |
| 1:AA:254:G:H1     | 1:AA:272:C:N4     | 2.11                     | 0.42              |
| 1:AA:454:C:N4     | 1:AA:479:C:N3     | 2.67                     | 0.42              |
| 1:AA:530:G:O2'    | 1:AA:531:U:P      | 2.76                     | 0.42              |
| 1:AA:546:G:H5'    | 1:AA:549:C:OP1    | 2.20                     | 0.42              |
| 1:AA:701:C:O2'    | 1:AA:703:G:C5     | 2.64                     | 0.42              |
| 1:AA:825:G:H2'    | 1:AA:826:C:H6     | 1.84                     | 0.42              |
| 1:AA:840:C:H4'    | 1:AA:841:U:OP1    | 2.18                     | 0.42              |
| 1:AA:923:A:C2     | 1:AA:924:C:C2     | 3.08                     | 0.42              |
| 1:AA:961:U:OP2    | 1:AA:1223:C:C1'   | 2.68                     | 0.42              |
| 2:AB:185:ILE:HG23 | 2:AB:199:TYR:O    | 2.20                     | 0.42              |
| 4:AD:20:TYR:CE2   | 4:AD:27:TYR:HE2   | 2.37                     | 0.42              |
| 5:AE:136:MET:O    | 5:AE:140:ARG:HB2  | 2.19                     | 0.42              |
| 8:AH:97:VAL:C     | 8:AH:99:GLU:N     | 2.72                     | 0.42              |
| 9:AI:56:LEU:HD23  | 9:AI:56:LEU:O     | 2.19                     | 0.42              |
| 10:AJ:38:ILE:HA   | 10:AJ:39:PRO:HD3  | 1.67                     | 0.42              |
| 10:AJ:54:PHE:CE1  | 10:AJ:55:LYS:HE3  | 2.55                     | 0.42              |
| 7:AG:151:TYR:OH   | 11:AK:54:ARG:HD3  | 2.19                     | 0.42              |
| 11:AK:65:ALA:O    | 11:AK:68:ALA:HB3  | 2.20                     | 0.42              |
| 12:AL:27:ALA:HA   | 12:AL:28:PRO:HD3  | 1.75                     | 0.42              |
| 12:AL:39:THR:HA   | 12:AL:50:ARG:O    | 2.20                     | 0.42              |
| 12:AL:56:ARG:HD3  | 12:AL:62:GLU:OE1  | 2.19                     | 0.42              |
| 10:AJ:46:ARG:NH1  | 14:AN:61:TRP:CZ2  | 2.88                     | 0.42              |
| 15:AO:14:GLU:HA   | 15:AO:14:GLU:OE1  | 2.19                     | 0.42              |
| 16:AP:26:ARG:HH11 | 16:AP:31:LYS:HB3  | 1.81                     | 0.42              |
| 17:AQ:29:HIS:ND1  | 17:AQ:29:HIS:C    | 2.73                     | 0.42              |
| 22:AV:9:G:N2      | 23:AW:34:U:C2     | 2.88                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AX:11:A:C6      | 24:AX:12:G:C6      | 3.07                     | 0.42              |
| 24:AX:16:C:O2'     | 24:AX:60:U:H4'     | 2.20                     | 0.42              |
| 50:B1:13:ILE:CG1   | 50:B1:42:GLN:HB2   | 2.50                     | 0.42              |
| 52:B3:46:ASN:O     | 52:B3:47:VAL:C     | 2.58                     | 0.42              |
| 27:BA:747:U:OP2    | 54:B5:3:LYS:HD3    | 2.19                     | 0.42              |
| 55:B6:11:LEU:CD1   | 55:B6:12:GLU:H     | 2.33                     | 0.42              |
| 57:B8:40:GLU:O     | 57:B8:43:GLN:N     | 2.47                     | 0.42              |
| 27:BA:111:A:C5     | 27:BA:112:U:C5     | 3.07                     | 0.42              |
| 27:BA:1322:A:C4    | 27:BA:1323:U:C5    | 3.08                     | 0.42              |
| 27:BA:1553:A:C8    | 27:BA:1555:G:C6    | 3.08                     | 0.42              |
| 27:BA:1437:C:H42   | 27:BA:1555:G:H1    | 1.68                     | 0.42              |
| 27:BA:1662:C:H2'   | 27:BA:1663:C:C6    | 2.55                     | 0.42              |
| 27:BA:1664:A:H2'   | 27:BA:1664:A:N3    | 2.34                     | 0.42              |
| 27:BA:1668:A:C8    | 27:BA:1674:G:C6    | 3.07                     | 0.42              |
| 27:BA:1776:G:N3    | 27:BA:1776:G:H2'   | 2.35                     | 0.42              |
| 27:BA:2438:U:O2    | 27:BA:2441:C:C4    | 2.72                     | 0.42              |
| 27:BA:258:G:N3     | 27:BA:259:G:C8     | 2.88                     | 0.42              |
| 27:BA:483:A:H2'    | 27:BA:484:C:C5'    | 2.50                     | 0.42              |
| 27:BA:485:C:O2'    | 27:BA:486:C:H5'    | 2.19                     | 0.42              |
| 27:BA:61:G:O2'     | 27:BA:62:C:O5'     | 2.36                     | 0.42              |
| 27:BA:761:A:H8     | 27:BA:761:A:O5'    | 2.03                     | 0.42              |
| 27:BA:769:G:H2'    | 27:BA:770:G:O5'    | 2.20                     | 0.42              |
| 27:BA:770:G:H8     | 27:BA:770:G:O5'    | 2.03                     | 0.42              |
| 27:BA:782:A:OP1    | 27:BA:783:A:N1     | 2.53                     | 0.42              |
| 28:BB:24:G:H1'     | 28:BB:27:C:N4      | 2.35                     | 0.42              |
| 30:BD:136:ILE:O    | 30:BD:137:PRO:C    | 2.57                     | 0.42              |
| 30:BD:147:LEU:HD12 | 30:BD:147:LEU:HA   | 1.74                     | 0.42              |
| 30:BD:21:PHE:CD1   | 30:BD:21:PHE:N     | 2.86                     | 0.42              |
| 30:BD:31:LYS:HD2   | 30:BD:33:LEU:CD1   | 2.46                     | 0.42              |
| 30:BD:32:SER:O     | 30:BD:34:VAL:N     | 2.40                     | 0.42              |
| 31:BE:63:LEU:C     | 31:BE:63:LEU:HD23  | 2.40                     | 0.42              |
| 32:BF:139:PHE:O    | 32:BF:142:TRP:HB3  | 2.18                     | 0.42              |
| 32:BF:113:ALA:CB   | 32:BF:186:ILE:HG21 | 2.48                     | 0.42              |
| 32:BF:37:VAL:HG13  | 32:BF:184:TYR:CD1  | 2.54                     | 0.42              |
| 33:BG:123:ASN:OD1  | 33:BG:123:ASN:N    | 2.53                     | 0.42              |
| 34:BH:10:PRO:HG3   | 34:BH:50:VAL:N     | 2.34                     | 0.42              |
| 34:BH:156:ALA:HB3  | 34:BH:159:GLU:HB2  | 2.02                     | 0.42              |
| 34:BH:158:HIS:CE1  | 34:BH:168:PRO:C    | 2.93                     | 0.42              |
| 36:BN:18:ALA:HB3   | 36:BN:26:LEU:HD22  | 2.00                     | 0.42              |
| 37:BO:24:VAL:HG22  | 37:BO:24:VAL:O     | 2.20                     | 0.42              |
| 39:BQ:97:VAL:HG11  | 39:BQ:103:MET:HE3  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BQ:118:LEU:HD12 | 39:BQ:131:ILE:CG2 | 2.50                     | 0.42              |
| 42:BT:101:PHE:O    | 42:BT:102:ILE:C   | 2.58                     | 0.42              |
| 45:BW:36:LEU:HD11  | 45:BW:47:VAL:HG12 | 2.02                     | 0.42              |
| 45:BW:7:ALA:O      | 45:BW:10:VAL:CG2  | 2.67                     | 0.42              |
| 47:BY:18:GLY:O     | 47:BY:20:TYR:N    | 2.52                     | 0.42              |
| 47:BY:30:VAL:HG13  | 47:BY:31:LEU:N    | 2.35                     | 0.42              |
| 1:CA:10:A:O2'      | 1:CA:11:G:H5'     | 2.20                     | 0.42              |
| 1:CA:1210:C:H4'    | 1:CA:1214:C:C5    | 2.54                     | 0.42              |
| 1:CA:960:U:C2      | 1:CA:1225:A:N7    | 2.88                     | 0.42              |
| 1:CA:1229:A:C2     | 1:CA:1230:C:C2    | 3.08                     | 0.42              |
| 1:CA:1258:G:O2'    | 1:CA:1259:C:C5'   | 2.68                     | 0.42              |
| 1:CA:1270:C:C2'    | 1:CA:1271:G:H5'   | 2.50                     | 0.42              |
| 1:CA:1286:A:H2'    | 1:CA:1287:A:O3'   | 2.19                     | 0.42              |
| 1:CA:1421:G:C6     | 1:CA:1422:G:C5    | 3.08                     | 0.42              |
| 1:CA:147:G:H2'     | 1:CA:148:G:H8     | 1.83                     | 0.42              |
| 1:CA:1521:G:H2'    | 1:CA:1522:U:H6    | 1.83                     | 0.42              |
| 1:CA:243:A:C5      | 1:CA:281:G:N2     | 2.87                     | 0.42              |
| 1:CA:282:A:H2'     | 1:CA:283:C:H6     | 1.85                     | 0.42              |
| 1:CA:422:C:C4'     | 1:CA:423:G:OP1    | 2.68                     | 0.42              |
| 1:CA:435:C:C2      | 1:CA:436:C:C5     | 3.08                     | 0.42              |
| 1:CA:62:U:H2'      | 1:CA:63:C:H6      | 1.85                     | 0.42              |
| 1:CA:818:G:H3'     | 1:CA:819:A:C5'    | 2.49                     | 0.42              |
| 1:CA:831:U:H2'     | 1:CA:832:C:C5'    | 2.48                     | 0.42              |
| 1:CA:914:A:H2'     | 1:CA:915:A:H8     | 1.85                     | 0.42              |
| 3:CC:138:VAL:CG2   | 3:CC:151:VAL:HG23 | 2.49                     | 0.42              |
| 4:CD:70:ILE:HD12   | 4:CD:100:ARG:NE   | 2.35                     | 0.42              |
| 5:CE:31:LEU:HD21   | 5:CE:43:LEU:HG    | 2.00                     | 0.42              |
| 6:CF:87:ARG:HG2    | 6:CF:87:ARG:HH11  | 1.85                     | 0.42              |
| 6:CF:91:VAL:HG12   | 6:CF:92:LYS:O     | 2.19                     | 0.42              |
| 7:CG:20:ASP:HB3    | 7:CG:23:VAL:CG2   | 2.44                     | 0.42              |
| 7:CG:50:ILE:O      | 7:CG:54:THR:HG23  | 2.20                     | 0.42              |
| 7:CG:73:MET:HA     | 7:CG:91:VAL:HG23  | 2.02                     | 0.42              |
| 8:CH:109:ILE:HG13  | 8:CH:122:ARG:HH12 | 1.85                     | 0.42              |
| 11:CK:33:THR:HB    | 11:CK:37:GLY:C    | 2.40                     | 0.42              |
| 11:CK:52:GLY:O     | 11:CK:55:LYS:HB2  | 2.20                     | 0.42              |
| 15:CO:2:PRO:HG2    | 15:CO:3:ILE:HD13  | 2.00                     | 0.42              |
| 16:CP:27:LYS:H     | 16:CP:27:LYS:HG2  | 1.42                     | 0.42              |
| 1:CA:128:G:H5'     | 17:CQ:2:PRO:O     | 2.20                     | 0.42              |
| 19:CS:42:PRO:O     | 19:CS:44:MET:SD   | 2.77                     | 0.42              |
| 24:CX:72:A:H5'     | 24:CX:73:A:OP2    | 2.19                     | 0.42              |
| 25:CY:49:G:HO2'    | 25:CY:50:A:P      | 2.43                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:D2:8:LYS:O      | 51:D2:9:GLN:C      | 2.58                     | 0.42              |
| 27:DA:1159:U:H2'   | 27:DA:1160:G:O4'   | 2.20                     | 0.42              |
| 27:DA:1309:G:C5'   | 56:D7:9:ARG:HG3    | 2.49                     | 0.42              |
| 27:DA:1449:A:H2'   | 27:DA:1449:A:N3    | 2.35                     | 0.42              |
| 27:DA:1669:A:H2'   | 27:DA:1669:A:N3    | 2.35                     | 0.42              |
| 27:DA:1695:G:O2'   | 27:DA:1696:G:O5'   | 2.37                     | 0.42              |
| 27:DA:1858:G:H2'   | 27:DA:1883:G:H22   | 1.83                     | 0.42              |
| 27:DA:1906:G:N2    | 27:DA:1907:G:C4    | 2.88                     | 0.42              |
| 27:DA:2048:G:H4'   | 27:DA:2823:A:C2    | 2.55                     | 0.42              |
| 27:DA:2053:G:C2'   | 27:DA:2054:A:H5'   | 2.50                     | 0.42              |
| 27:DA:214:G:H21    | 27:DA:216:A:H1'    | 1.85                     | 0.42              |
| 27:DA:2287:A:H62   | 27:DA:2344:U:H3    | 1.68                     | 0.42              |
| 27:DA:243:U:C2'    | 27:DA:244:A:H5'    | 2.50                     | 0.42              |
| 27:DA:2499:C:C4    | 27:DA:2500:U:C2    | 3.08                     | 0.42              |
| 27:DA:2611:U:HO2'  | 27:DA:2612:C:P     | 2.42                     | 0.42              |
| 27:DA:2723:C:OP2   | 31:DE:109:LYS:NZ   | 2.49                     | 0.42              |
| 27:DA:310:A:C4     | 27:DA:312:G:N7     | 2.88                     | 0.42              |
| 27:DA:40:C:H42     | 27:DA:438:G:H1     | 1.67                     | 0.42              |
| 27:DA:510:C:OP1    | 27:DA:511:U:OP2    | 2.38                     | 0.42              |
| 27:DA:13:A:C2      | 27:DA:526:A:C5     | 3.08                     | 0.42              |
| 27:DA:775:G:P      | 27:DA:777:A:H1'    | 2.60                     | 0.42              |
| 27:DA:784:A:C6     | 27:DA:792:G:O4'    | 2.73                     | 0.42              |
| 27:DA:817:C:O2'    | 27:DA:818:G:H5'    | 2.20                     | 0.42              |
| 28:DB:85:G:H2'     | 28:DB:86:G:H8      | 1.85                     | 0.42              |
| 30:DD:111:LEU:C    | 30:DD:111:LEU:HD13 | 2.40                     | 0.42              |
| 27:DA:2579:C:H4'   | 31:DE:134:ILE:HD12 | 2.01                     | 0.42              |
| 31:DE:167:VAL:HG21 | 31:DE:170:LEU:HD11 | 2.02                     | 0.42              |
| 32:DF:115:ALA:O    | 32:DF:116:ASP:C    | 2.58                     | 0.42              |
| 32:DF:70:THR:OG1   | 32:DF:71:GLY:N     | 2.52                     | 0.42              |
| 34:DH:102:ALA:CA   | 34:DH:117:PRO:HD3  | 2.47                     | 0.42              |
| 35:DI:116:LEU:O    | 35:DI:117:GLU:O    | 2.36                     | 0.42              |
| 36:DN:34:LEU:O     | 36:DN:116:LEU:HD22 | 2.19                     | 0.42              |
| 36:DN:128:HIS:HA   | 36:DN:129:PRO:HD2  | 1.88                     | 0.42              |
| 36:DN:79:PRO:C     | 36:DN:81:GLY:N     | 2.73                     | 0.42              |
| 41:DS:78:LEU:CD1   | 41:DS:103:GLU:HB3  | 2.44                     | 0.42              |
| 41:DS:31:SER:O     | 41:DS:34:HIS:N     | 2.36                     | 0.42              |
| 43:DU:109:LEU:HA   | 43:DU:109:LEU:HD23 | 1.84                     | 0.42              |
| 45:DW:90:ARG:HH11  | 45:DW:90:ARG:HG3   | 1.85                     | 0.42              |
| 47:DY:87:LYS:NZ    | 47:DY:89:PHE:CE1   | 2.88                     | 0.42              |
| 1:AA:1081:G:C2     | 1:AA:1082:G:C8     | 3.08                     | 0.42              |
| 1:AA:1268:A:H4'    | 21:AU:20:LYS:N     | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:321:A:H4'    | 1:AA:1435:G:O2'   | 2.20                     | 0.42              |
| 1:AA:14:U:O2      | 1:AA:16:A:H3'     | 2.20                     | 0.42              |
| 1:AA:389:A:H2'    | 1:AA:390:C:O4'    | 2.20                     | 0.42              |
| 1:AA:456:C:H2'    | 1:AA:457:C:C6     | 2.55                     | 0.42              |
| 1:AA:673:G:N2     | 1:AA:674:G:C2     | 2.88                     | 0.42              |
| 1:AA:730:G:C6     | 1:AA:731:G:H1'    | 2.55                     | 0.42              |
| 1:AA:825:G:N1     | 1:AA:876:G:C6     | 2.88                     | 0.42              |
| 1:AA:995:C:H6     | 1:AA:995:C:O5'    | 2.03                     | 0.42              |
| 2:AB:188:ALA:O    | 2:AB:203:GLY:N    | 2.44                     | 0.42              |
| 4:AD:195:ALA:O    | 4:AD:196:LEU:C    | 2.58                     | 0.42              |
| 5:AE:102:ALA:O    | 5:AE:107:ARG:NH1  | 2.53                     | 0.42              |
| 5:AE:33:VAL:HG21  | 5:AE:109:ILE:HD11 | 2.01                     | 0.42              |
| 7:AG:49:ILE:HG22  | 7:AG:49:ILE:O     | 2.19                     | 0.42              |
| 8:AH:14:ARG:C     | 8:AH:16:ALA:N     | 2.73                     | 0.42              |
| 9:AI:14:VAL:HG12  | 9:AI:15:ALA:N     | 2.35                     | 0.42              |
| 10:AJ:79:ARG:O    | 10:AJ:80:LYS:C    | 2.57                     | 0.42              |
| 13:AM:15:VAL:CG2  | 13:AM:16:ASP:N    | 2.83                     | 0.42              |
| 10:AJ:63:PHE:HB3  | 14:AN:59:ALA:H    | 1.85                     | 0.42              |
| 19:AS:33:THR:OG1  | 19:AS:34:TRP:N    | 2.53                     | 0.42              |
| 20:AT:61:SER:O    | 20:AT:65:LYS:HB2  | 2.20                     | 0.42              |
| 23:AW:60:C:H2'    | 23:AW:61:C:C6     | 2.55                     | 0.42              |
| 50:B1:13:ILE:HD11 | 50:B1:42:GLN:OE1  | 2.20                     | 0.42              |
| 51:B2:50:ILE:C    | 51:B2:52:ASP:N    | 2.73                     | 0.42              |
| 52:B3:23:LEU:O    | 52:B3:27:GLY:N    | 2.52                     | 0.42              |
| 53:B4:40:ILE:HA   | 53:B4:57:ILE:CG2  | 2.49                     | 0.42              |
| 27:BA:1175:U:P    | 27:BA:1176:G:H5'  | 2.59                     | 0.42              |
| 27:BA:1451:C:H2'  | 27:BA:1451:C:O2   | 2.19                     | 0.42              |
| 27:BA:1505:C:HO2' | 27:BA:1506:C:P    | 2.43                     | 0.42              |
| 27:BA:1524:G:N2   | 27:BA:1525:G:H1'  | 2.35                     | 0.42              |
| 27:BA:1296:G:N2   | 27:BA:1645:G:C4   | 2.88                     | 0.42              |
| 27:BA:1750:G:C2   | 27:BA:1751:C:C2   | 3.08                     | 0.42              |
| 27:BA:1783:A:C2   | 27:BA:2587:A:C5   | 3.08                     | 0.42              |
| 27:BA:1884:A:C3'  | 27:BA:1885:A:H5'' | 2.48                     | 0.42              |
| 27:BA:1899:G:N2   | 27:BA:1903:G:C5   | 2.87                     | 0.42              |
| 27:BA:193:U:O2'   | 27:BA:194:G:H5'   | 2.20                     | 0.42              |
| 27:BA:1900:A:H1'  | 27:BA:1970:A:H2'  | 2.01                     | 0.42              |
| 27:BA:2337:G:C2   | 27:BA:2338:G:C5   | 3.08                     | 0.42              |
| 27:BA:2371:G:H4'  | 55:B6:45:LYS:HB3  | 2.02                     | 0.42              |
| 27:BA:2406:U:H4'  | 27:BA:2407:G:O5'  | 2.20                     | 0.42              |
| 27:BA:2246:G:H1'  | 27:BA:2426:A:C2   | 2.55                     | 0.42              |
| 27:BA:2471:C:H2'  | 27:BA:2471:C:O2   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BA:2447:G:O2'  | 27:BA:2500:U:OP2  | 2.24                     | 0.42              |
| 27:BA:2725:A:O2'  | 27:BA:2726:U:O5'  | 2.36                     | 0.42              |
| 27:BA:321:G:O3'   | 27:BA:322:A:H8    | 2.03                     | 0.42              |
| 27:BA:13:A:C2     | 27:BA:526:A:N7    | 2.88                     | 0.42              |
| 27:BA:644:A:H4'   | 27:BA:645:C:H5    | 1.81                     | 0.42              |
| 27:BA:706:A:C5    | 27:BA:707:G:C8    | 3.08                     | 0.42              |
| 28:BB:47:C:O2'    | 28:BB:48:A:H5'    | 2.20                     | 0.42              |
| 29:BC:214:VAL:O   | 29:BC:216:THR:N   | 2.53                     | 0.42              |
| 31:BE:3:GLY:O     | 31:BE:4:ILE:CB    | 2.64                     | 0.42              |
| 32:BF:116:ASP:OD2 | 38:BP:5:ASP:HB2   | 2.20                     | 0.42              |
| 32:BF:157:VAL:HB  | 32:BF:194:MET:HB3 | 2.01                     | 0.42              |
| 33:BG:84:LYS:HB3  | 33:BG:85:GLY:H    | 1.62                     | 0.42              |
| 35:BI:25:TYR:CD1  | 35:BI:30:LEU:HD11 | 2.55                     | 0.42              |
| 37:BO:59:LYS:HZ3  | 37:BO:89:ASN:HD21 | 1.68                     | 0.42              |
| 41:BS:106:ARG:NE  | 41:BS:107:GLU:O   | 2.53                     | 0.42              |
| 41:BS:46:VAL:HG12 | 41:BS:47:THR:O    | 2.19                     | 0.42              |
| 41:BS:90:GLY:O    | 41:BS:92:TYR:HD1  | 2.03                     | 0.42              |
| 42:BT:9:LEU:C     | 42:BT:11:GLU:N    | 2.74                     | 0.42              |
| 44:BV:91:TYR:O    | 44:BV:92:THR:CG2  | 2.66                     | 0.42              |
| 45:BW:41:LYS:C    | 45:BW:43:GLY:N    | 2.72                     | 0.42              |
| 45:BW:97:LYS:HE3  | 45:BW:99:ARG:NH1  | 2.34                     | 0.42              |
| 1:CA:1098:C:C4    | 1:CA:1099:G:C8    | 3.08                     | 0.42              |
| 1:CA:1152:A:H5'   | 10:CJ:70:ARG:HH22 | 1.84                     | 0.42              |
| 1:CA:1273:G:C5    | 1:CA:1274:G:C5    | 3.08                     | 0.42              |
| 1:CA:1283:G:H2'   | 1:CA:1284:C:H6    | 1.85                     | 0.42              |
| 1:CA:1260:C:OP1   | 1:CA:1284:C:H4'   | 2.19                     | 0.42              |
| 1:CA:1478:C:H2'   | 1:CA:1479:C:C6    | 2.50                     | 0.42              |
| 1:CA:1508:G:H2'   | 1:CA:1509:C:C6    | 2.55                     | 0.42              |
| 1:CA:151:A:H2'    | 1:CA:152:A:O4'    | 2.20                     | 0.42              |
| 1:CA:309:G:O2'    | 1:CA:310:G:H5'    | 2.20                     | 0.42              |
| 1:CA:126:G:H5'    | 1:CA:633:G:N2     | 2.35                     | 0.42              |
| 1:CA:679:C:O2'    | 1:CA:680:C:H5'    | 2.20                     | 0.42              |
| 1:CA:705:U:C5     | 1:CA:706:A:C5     | 3.08                     | 0.42              |
| 1:CA:750:G:H21    | 15:CO:23:GLY:CA   | 2.33                     | 0.42              |
| 1:CA:860:A:C8     | 1:CA:861:G:C8     | 3.07                     | 0.42              |
| 1:CA:884:U:H4'    | 1:CA:885:G:H5''   | 2.01                     | 0.42              |
| 1:CA:891:U:H2'    | 1:CA:892:A:H8     | 1.85                     | 0.42              |
| 2:CB:131:PRO:O    | 2:CB:135:GLN:HG3  | 2.20                     | 0.42              |
| 2:CB:59:GLU:O     | 2:CB:62:ALA:HB3   | 2.19                     | 0.42              |
| 6:CF:12:PRO:HB3   | 6:CF:58:GLY:CA    | 2.50                     | 0.42              |
| 8:CH:111:ILE:CG2  | 8:CH:112:LEU:H    | 2.24                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:9:MET:O       | 8:CH:12:ARG:HB3    | 2.20                     | 0.42              |
| 11:CK:20:TYR:C     | 11:CK:21:ILE:HD12  | 2.40                     | 0.42              |
| 11:CK:52:GLY:N     | 11:CK:55:LYS:HG3   | 2.35                     | 0.42              |
| 13:CM:14:ARG:NH2   | 13:CM:42:ALA:HA    | 2.35                     | 0.42              |
| 13:CM:70:LEU:HD23  | 13:CM:71:ARG:H     | 1.80                     | 0.42              |
| 1:CA:1308:U:O3'    | 13:CM:92:HIS:HE1   | 2.03                     | 0.42              |
| 14:CN:26:ARG:HD2   | 14:CN:43:CYS:CB    | 2.49                     | 0.42              |
| 15:CO:8:LYS:O      | 15:CO:12:ILE:HG13  | 2.20                     | 0.42              |
| 15:CO:65:ARG:HH11  | 15:CO:65:ARG:HG2   | 1.85                     | 0.42              |
| 17:CQ:64:PRO:HG3   | 17:CQ:70:ARG:HG2   | 2.02                     | 0.42              |
| 18:CR:76:LEU:N     | 18:CR:76:LEU:HD22  | 2.35                     | 0.42              |
| 19:CS:52:TYR:HE1   | 19:CS:56:GLN:HA    | 1.83                     | 0.42              |
| 23:CW:2:G:C2       | 23:CW:71:A:C2      | 3.08                     | 0.42              |
| 50:D1:23:LYS:HE2   | 50:D1:28:GLY:N     | 2.35                     | 0.42              |
| 50:D1:56:GLN:NE2   | 50:D1:56:GLN:HA    | 2.34                     | 0.42              |
| 52:D3:33:GLN:C     | 52:D3:34:GLU:HG3   | 2.40                     | 0.42              |
| 57:D8:63:PRO:O     | 57:D8:64:TYR:C     | 2.58                     | 0.42              |
| 27:DA:1109:C:H5''  | 27:DA:1110:G:OP2   | 2.20                     | 0.42              |
| 27:DA:1200:C:H2'   | 27:DA:1201:C:C6    | 2.55                     | 0.42              |
| 27:DA:1210:A:H1'   | 27:DA:1212:G:C4    | 2.54                     | 0.42              |
| 27:DA:1261:C:C2'   | 27:DA:1262:A:O5'   | 2.68                     | 0.42              |
| 27:DA:175:G:C5     | 27:DA:176:G:N7     | 2.88                     | 0.42              |
| 27:DA:1815:A:O2'   | 27:DA:1816:G:O5'   | 2.35                     | 0.42              |
| 27:DA:1847:A:P     | 27:DA:1847:A:O4'   | 2.78                     | 0.42              |
| 27:DA:1652:A:C2    | 27:DA:2006:C:N3    | 2.88                     | 0.42              |
| 27:DA:2189:U:H3'   | 27:DA:2190:G:H5''  | 2.02                     | 0.42              |
| 27:DA:2399:G:C6    | 27:DA:2418:A:C6    | 3.08                     | 0.42              |
| 27:DA:2709:G:H2'   | 27:DA:2710:C:O4'   | 2.20                     | 0.42              |
| 27:DA:2711:A:N6    | 27:DA:2714:G:C5    | 2.88                     | 0.42              |
| 27:DA:2850:A:H2'   | 27:DA:2851:A:C8    | 2.55                     | 0.42              |
| 27:DA:2850:A:H2'   | 27:DA:2851:A:H8    | 1.84                     | 0.42              |
| 27:DA:300:A:N6     | 27:DA:334:C:H5'    | 2.35                     | 0.42              |
| 27:DA:534:U:O2'    | 43:DU:49:HIS:CD2   | 2.71                     | 0.42              |
| 27:DA:574:C:O3'    | 27:DA:2055:C:C5    | 2.73                     | 0.42              |
| 27:DA:636:G:OP2    | 38:DP:113:LYS:NZ   | 2.34                     | 0.42              |
| 27:DA:811:U:OP2    | 38:DP:24:GLY:CA    | 2.67                     | 0.42              |
| 27:DA:847:U:N3     | 27:DA:934:G:N2     | 2.68                     | 0.42              |
| 27:DA:857:C:C5'    | 49:D0:77:ARG:HH22  | 2.32                     | 0.42              |
| 29:DC:99:ILE:HG23  | 29:DC:110:PHE:CB   | 2.50                     | 0.42              |
| 30:DD:147:LEU:CD2  | 30:DD:155:LEU:HD11 | 2.50                     | 0.42              |
| 30:DD:173:VAL:HG23 | 30:DD:174:ILE:N    | 2.35                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DF:22:ALA:O     | 32:DF:24:LEU:O    | 2.37                     | 0.42              |
| 33:DG:45:GLU:C     | 33:DG:47:LYS:H    | 2.22                     | 0.42              |
| 34:DH:166:GLY:C    | 34:DH:167:GLU:OE1 | 2.58                     | 0.42              |
| 35:DI:138:ILE:HG13 | 35:DI:139:GLN:N   | 2.24                     | 0.42              |
| 36:DN:87:LEU:HD23  | 36:DN:87:LEU:C    | 2.40                     | 0.42              |
| 39:DQ:51:ARG:CG    | 39:DQ:51:ARG:HH11 | 2.33                     | 0.42              |
| 40:DR:38:VAL:HG12  | 40:DR:39:PRO:N    | 2.34                     | 0.42              |
| 42:DT:11:GLU:C     | 42:DT:13:ARG:N    | 2.73                     | 0.42              |
| 37:DO:78:ARG:NE    | 42:DT:73:GLU:OE2  | 2.53                     | 0.42              |
| 44:DV:12:TYR:CE2   | 44:DV:22:VAL:CG1  | 3.03                     | 0.42              |
| 47:DY:27:VAL:C     | 47:DY:28:LYS:HD3  | 2.40                     | 0.42              |
| 47:DY:28:LYS:HA    | 47:DY:38:ILE:HB   | 2.02                     | 0.42              |
| 47:DY:54:LYS:HZ3   | 47:DY:55:TYR:HE2  | 1.65                     | 0.42              |
| 1:AA:1147:C:O2'    | 1:AA:1148:U:H5'   | 2.19                     | 0.42              |
| 1:AA:1240:U:H3'    | 1:AA:1241:G:H5'   | 2.01                     | 0.42              |
| 1:AA:1284:C:H3'    | 1:AA:1285:A:H8    | 1.83                     | 0.42              |
| 1:AA:1360:A:H2'    | 1:AA:1361:G:O4'   | 2.20                     | 0.42              |
| 1:AA:137:C:C2'     | 1:AA:138:G:H5'    | 2.50                     | 0.42              |
| 1:AA:1401:G:C2     | 1:AA:1402:C:H1'   | 2.55                     | 0.42              |
| 1:AA:261:U:H2'     | 1:AA:263:A:C8     | 2.55                     | 0.42              |
| 1:AA:113:G:C1'     | 1:AA:354:G:H5'    | 2.49                     | 0.42              |
| 1:AA:383:A:H2'     | 1:AA:384:G:C5'    | 2.50                     | 0.42              |
| 1:AA:451:A:O4'     | 1:AA:452:A:N7     | 2.52                     | 0.42              |
| 1:AA:578:C:O2'     | 1:AA:579:G:O5'    | 2.37                     | 0.42              |
| 1:AA:643:C:C2      | 1:AA:644:G:C8     | 3.08                     | 0.42              |
| 1:AA:728:A:C8      | 15:AO:54:ARG:NE   | 2.87                     | 0.42              |
| 1:AA:911:U:C2      | 1:AA:912:C:C5     | 3.08                     | 0.42              |
| 1:AA:92:C:H2'      | 1:AA:93:G:H8      | 1.84                     | 0.42              |
| 3:AC:142:MET:HG3   | 3:AC:170:GLN:NE2  | 2.34                     | 0.42              |
| 3:AC:51:GLY:C      | 3:AC:52:LEU:HD23  | 2.40                     | 0.42              |
| 5:AE:148:VAL:HG12  | 5:AE:149:GLU:N    | 2.34                     | 0.42              |
| 6:AF:2:ARG:HD3     | 6:AF:4:TYR:OH     | 2.20                     | 0.42              |
| 7:AG:27:ILE:HG22   | 7:AG:39:ALA:CB    | 2.49                     | 0.42              |
| 13:AM:49:THR:HG1   | 13:AM:52:GLU:HG3  | 1.84                     | 0.42              |
| 13:AM:52:GLU:HA    | 13:AM:55:ARG:HH21 | 1.83                     | 0.42              |
| 14:AN:17:LYS:HG3   | 14:AN:17:LYS:O    | 2.20                     | 0.42              |
| 15:AO:38:ARG:NH1   | 15:AO:38:ARG:CG   | 2.81                     | 0.42              |
| 15:AO:4:THR:O      | 15:AO:7:GLU:HB2   | 2.20                     | 0.42              |
| 18:AR:87:ARG:O     | 18:AR:87:ARG:HG2  | 2.20                     | 0.42              |
| 20:AT:54:LYS:HA    | 20:AT:57:ARG:CZ   | 2.50                     | 0.42              |
| 50:B1:51:VAL:CG1   | 50:B1:51:VAL:O    | 2.68                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1042:G:H3'  | 27:BA:1043:C:O4'   | 2.20                     | 0.42              |
| 27:BA:1212:G:C2   | 27:BA:1236:G:C5    | 3.08                     | 0.42              |
| 27:BA:1398:C:C2'  | 27:BA:1399:C:H5'   | 2.50                     | 0.42              |
| 27:BA:1761:C:H3'  | 27:BA:1762:A:H8    | 1.83                     | 0.42              |
| 27:BA:2206:G:N3   | 27:BA:2206:G:H3'   | 2.35                     | 0.42              |
| 27:BA:2245:U:C5'  | 27:BA:2246:G:H5'   | 2.50                     | 0.42              |
| 27:BA:2320:A:C2'  | 27:BA:2320:A:N3    | 2.81                     | 0.42              |
| 27:BA:2453:A:H2'  | 27:BA:2454:G:H8    | 1.85                     | 0.42              |
| 27:BA:2662:A:H2'  | 27:BA:2663:G:O4'   | 2.20                     | 0.42              |
| 27:BA:2676:C:H2'  | 27:BA:2677:G:H8    | 1.85                     | 0.42              |
| 27:BA:2807:G:H1   | 27:BA:2892:A:H62   | 1.68                     | 0.42              |
| 27:BA:31:C:O2'    | 27:BA:32:C:H5'     | 2.19                     | 0.42              |
| 27:BA:431:U:O5'   | 27:BA:431:U:C6     | 2.72                     | 0.42              |
| 27:BA:675:A:C5    | 27:BA:676:A:C6     | 3.08                     | 0.42              |
| 27:BA:92:A:O2'    | 27:BA:93:G:C8      | 2.73                     | 0.42              |
| 28:BB:13:A:N1     | 28:BB:69:G:O2'     | 2.44                     | 0.42              |
| 30:BD:126:GLN:HG2 | 30:BD:129:ASN:ND2  | 2.34                     | 0.42              |
| 30:BD:4:LYS:HD2   | 30:BD:18:VAL:HG23  | 2.02                     | 0.42              |
| 31:BE:116:VAL:O   | 31:BE:117:MET:CB   | 2.56                     | 0.42              |
| 32:BF:161:GLU:O   | 32:BF:165:ARG:HG3  | 2.20                     | 0.42              |
| 32:BF:183:VAL:HA  | 32:BF:186:ILE:HB   | 2.02                     | 0.42              |
| 32:BF:64:ILE:HG23 | 32:BF:65:TRP:CG    | 2.54                     | 0.42              |
| 34:BH:111:HIS:HA  | 34:BH:112:PRO:HD2  | 1.68                     | 0.42              |
| 34:BH:12:PRO:HD2  | 34:BH:49:VAL:HG12  | 2.02                     | 0.42              |
| 37:BO:97:ARG:HA   | 37:BO:117:LEU:HD21 | 2.01                     | 0.42              |
| 40:BR:39:PRO:O    | 40:BR:40:LYS:C     | 2.58                     | 0.42              |
| 40:BR:44:LEU:HD13 | 40:BR:48:VAL:CG2   | 2.50                     | 0.42              |
| 40:BR:4:LEU:C     | 40:BR:6:SER:N      | 2.71                     | 0.42              |
| 40:BR:83:ILE:O    | 40:BR:86:ARG:HG3   | 2.19                     | 0.42              |
| 41:BS:37:ALA:O    | 41:BS:73:LEU:HD11  | 2.20                     | 0.42              |
| 41:BS:53:SER:O    | 41:BS:55:ALA:N     | 2.53                     | 0.42              |
| 41:BS:65:VAL:HG12 | 41:BS:66:ALA:N     | 2.34                     | 0.42              |
| 42:BT:53:ARG:HG2  | 42:BT:53:ARG:HH11  | 1.85                     | 0.42              |
| 44:BV:92:THR:OG1  | 44:BV:92:THR:O     | 2.38                     | 0.42              |
| 46:BX:12:VAL:HG12 | 46:BX:27:THR:CG2   | 2.50                     | 0.42              |
| 1:CA:1009:G:H22   | 1:CA:1021:G:H1'    | 1.85                     | 0.42              |
| 1:CA:1066:C:H2'   | 1:CA:1067:A:H8     | 1.83                     | 0.42              |
| 1:CA:1072:G:C5    | 1:CA:1073:U:C4     | 3.08                     | 0.42              |
| 1:CA:1159:U:C4    | 1:CA:1182:G:C5     | 3.08                     | 0.42              |
| 1:CA:1118:C:H1'   | 1:CA:1179:A:C5     | 2.54                     | 0.42              |
| 1:CA:323:U:C6     | 1:CA:323:U:H3'     | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:472:A:H1'    | 16:CP:82:GLN:OE1  | 2.20                     | 0.42              |
| 1:CA:548:G:O2'    | 1:CA:549:C:H5'    | 2.20                     | 0.42              |
| 1:CA:862:C:C2     | 1:CA:863:U:C5     | 3.07                     | 0.42              |
| 1:CA:913:A:H1'    | 1:CA:914:A:C1'    | 2.50                     | 0.42              |
| 1:CA:974:A:C8     | 1:CA:974:A:OP1    | 2.73                     | 0.42              |
| 1:CA:961:U:C4     | 1:CA:983:A:N6     | 2.87                     | 0.42              |
| 4:CD:105:VAL:HG21 | 4:CD:126:ILE:HG13 | 2.01                     | 0.42              |
| 4:CD:14:ARG:C     | 4:CD:16:GLY:H     | 2.23                     | 0.42              |
| 5:CE:50:GLU:O     | 5:CE:54:ALA:HB2   | 2.20                     | 0.42              |
| 6:CF:8:ILE:CG2    | 6:CF:10:LEU:HD11  | 2.39                     | 0.42              |
| 9:CI:40:LEU:C     | 9:CI:42:ARG:N     | 2.71                     | 0.42              |
| 10:CJ:8:LEU:HD23  | 10:CJ:8:LEU:HA    | 1.74                     | 0.42              |
| 13:CM:37:THR:O    | 13:CM:55:ARG:NH2  | 2.52                     | 0.42              |
| 17:CQ:5:VAL:HG12  | 17:CQ:5:VAL:O     | 2.19                     | 0.42              |
| 19:CS:33:THR:HG23 | 19:CS:51:VAL:HA   | 2.02                     | 0.42              |
| 20:CT:25:ARG:HG2  | 20:CT:29:LYS:HE3  | 2.01                     | 0.42              |
| 21:CU:9:ARG:O     | 21:CU:13:ILE:HG13 | 2.20                     | 0.42              |
| 24:CX:30:G:C6     | 24:CX:31:G:N7     | 2.88                     | 0.42              |
| 24:CX:44:A:O2'    | 24:CX:45:G:H5'    | 2.19                     | 0.42              |
| 25:CY:24:C:H2'    | 25:CY:25:A:C8     | 2.53                     | 0.42              |
| 52:D3:39:ASP:CG   | 52:D3:44:ARG:NE   | 2.73                     | 0.42              |
| 27:DA:254:G:H22   | 57:D8:8:LYS:HZ1   | 1.67                     | 0.42              |
| 58:D9:24:TYR:HB3  | 58:D9:25:VAL:H    | 1.66                     | 0.42              |
| 27:DA:1042:G:H5'' | 27:DA:1043:C:H6   | 1.81                     | 0.42              |
| 27:DA:1140:C:H1'  | 27:DA:1143:A:C2   | 2.55                     | 0.42              |
| 27:DA:1180:C:H2'  | 27:DA:1181:C:H5'  | 2.02                     | 0.42              |
| 27:DA:1268:A:C2'  | 27:DA:1269:A:H5'  | 2.50                     | 0.42              |
| 27:DA:1334:G:C6   | 27:DA:1335:U:C4   | 3.08                     | 0.42              |
| 27:DA:1338:G:C6   | 27:DA:1339:G:N7   | 2.88                     | 0.42              |
| 27:DA:1495:A:C8   | 27:DA:1495:A:OP1  | 2.73                     | 0.42              |
| 27:DA:1709:U:H2'  | 27:DA:1710:C:C6   | 2.55                     | 0.42              |
| 27:DA:1750:G:O2'  | 27:DA:1751:C:H5'  | 2.20                     | 0.42              |
| 27:DA:1793:C:C2   | 27:DA:1794:U:C5   | 3.08                     | 0.42              |
| 27:DA:17:G:H1     | 27:DA:523:C:N4    | 2.15                     | 0.42              |
| 27:DA:2297:C:H2'  | 27:DA:2298:A:H8   | 1.83                     | 0.42              |
| 27:DA:2349:G:OP2  | 57:D8:42:ARG:NH2  | 2.49                     | 0.42              |
| 27:DA:2413:G:H2'  | 27:DA:2414:G:H8   | 1.85                     | 0.42              |
| 27:DA:2554:U:C6   | 27:DA:2555:U:C5   | 2.94                     | 0.42              |
| 27:DA:2615:U:H6   | 27:DA:2615:U:O5'  | 2.03                     | 0.42              |
| 27:DA:2652:C:H42  | 27:DA:2668:G:H1   | 1.67                     | 0.42              |
| 27:DA:271(D):G:C6 | 27:DA:271(E):U:C4 | 3.08                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:2741:A:N6   | 27:DA:2763:G:O2'   | 2.47                     | 0.42              |
| 27:DA:412:A:N6    | 27:DA:2412:A:O4'   | 2.53                     | 0.42              |
| 27:DA:522:G:C4    | 27:DA:523:C:C6     | 3.08                     | 0.42              |
| 27:DA:552:G:C2'   | 27:DA:553:G:H5'    | 2.50                     | 0.42              |
| 27:DA:590:A:H2'   | 27:DA:591:C:C6     | 2.54                     | 0.42              |
| 27:DA:695:G:C4    | 27:DA:768:G:C6     | 3.08                     | 0.42              |
| 27:DA:999:U:O2    | 27:DA:999:U:C2'    | 2.67                     | 0.42              |
| 29:DC:38:ASP:HB2  | 29:DC:181:PRO:CB   | 2.50                     | 0.42              |
| 30:DD:183:ARG:HG2 | 30:DD:184:LYS:O    | 2.20                     | 0.42              |
| 30:DD:247:ALA:HA  | 30:DD:254:THR:HG22 | 2.01                     | 0.42              |
| 30:DD:35:LYS:HA   | 30:DD:35:LYS:HD3   | 1.75                     | 0.42              |
| 27:DA:1568:G:C5'  | 30:DD:61:LEU:HB2   | 2.50                     | 0.42              |
| 30:DD:72:LYS:HE2  | 30:DD:101:GLU:CD   | 2.40                     | 0.42              |
| 31:DE:14:ILE:HD11 | 31:DE:173:VAL:HG11 | 2.00                     | 0.42              |
| 31:DE:151:TYR:O   | 31:DE:152:LYS:C    | 2.58                     | 0.42              |
| 31:DE:16:ARG:C    | 31:DE:18:ASP:N     | 2.72                     | 0.42              |
| 32:DF:203:GLN:O   | 32:DF:206:ILE:HG13 | 2.20                     | 0.42              |
| 33:DG:178:PHE:HA  | 33:DG:179:PRO:HD3  | 1.68                     | 0.42              |
| 33:DG:180:PHE:C   | 33:DG:182:LYS:N    | 2.72                     | 0.42              |
| 33:DG:73:ALA:HB3  | 33:DG:85:GLY:O     | 2.20                     | 0.42              |
| 34:DH:97:ARG:O    | 34:DH:125:VAL:HG21 | 2.20                     | 0.42              |
| 34:DH:127:GLU:C   | 34:DH:129:THR:N    | 2.72                     | 0.42              |
| 34:DH:43:VAL:HG23 | 34:DH:43:VAL:O     | 2.20                     | 0.42              |
| 35:DI:117:GLU:O   | 35:DI:118:LYS:C    | 2.59                     | 0.42              |
| 36:DN:75:TYR:CD1  | 36:DN:81:GLY:O     | 2.73                     | 0.42              |
| 37:DO:20:MET:O    | 37:DO:41:ALA:HA    | 2.20                     | 0.42              |
| 38:DP:99:LEU:HG   | 38:DP:102:ARG:HH11 | 1.84                     | 0.42              |
| 42:DT:23:ARG:HB2  | 42:DT:120:ARG:NH1  | 2.35                     | 0.42              |
| 42:DT:27:THR:C    | 42:DT:28:VAL:HG23  | 2.40                     | 0.42              |
| 43:DU:80:ILE:HG22 | 43:DU:81:HIS:N     | 2.34                     | 0.42              |
| 44:DV:21:ARG:H    | 44:DV:21:ARG:HD3   | 1.83                     | 0.42              |
| 45:DW:50:VAL:HG22 | 45:DW:51:LEU:N     | 2.35                     | 0.42              |
| 45:DW:1:MET:HB3   | 45:DW:64:MET:HE3   | 2.01                     | 0.42              |
| 47:DY:11:ASP:HB2  | 47:DY:12:THR:H     | 1.64                     | 0.42              |
| 48:DZ:119:ILE:O   | 48:DZ:170:ILE:CA   | 2.65                     | 0.42              |
| 48:DZ:120:HIS:O   | 48:DZ:122:ASP:N    | 2.53                     | 0.42              |
| 48:DZ:150:HIS:HB3 | 48:DZ:169:THR:CB   | 2.50                     | 0.42              |
| 48:DZ:96:GLU:O    | 48:DZ:97:MET:HB3   | 2.20                     | 0.42              |
| 1:AA:1126:U:O2'   | 1:AA:1127:G:C5'    | 2.67                     | 0.41              |
| 1:AA:1145:C:C4'   | 1:AA:1146:A:OP1    | 2.68                     | 0.41              |
| 1:AA:1221:G:H2'   | 1:AA:1222:G:H8     | 1.85                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:AA:1410:G:H2'    | 1:AA:1411:C:C6      | 2.54                     | 0.41              |
| 1:AA:155:C:O2      | 1:AA:167:G:N2       | 2.53                     | 0.41              |
| 1:AA:278:G:OP2     | 17:AQ:41:LYS:NZ     | 2.53                     | 0.41              |
| 1:AA:62:U:H2'      | 1:AA:63:C:C6        | 2.54                     | 0.41              |
| 1:AA:67:C:H2'      | 1:AA:68:G:C8        | 2.54                     | 0.41              |
| 1:AA:687:A:C2      | 1:AA:704:A:C6       | 3.08                     | 0.41              |
| 1:AA:8:A:N7        | 4:AD:208:SER:CB     | 2.79                     | 0.41              |
| 2:AB:12:GLU:HG3    | 2:AB:12:GLU:H       | 1.63                     | 0.41              |
| 2:AB:80:ILE:O      | 2:AB:81:VAL:C       | 2.58                     | 0.41              |
| 3:AC:134:ILE:C     | 3:AC:136:GLN:N      | 2.72                     | 0.41              |
| 3:AC:139:GLN:O     | 3:AC:143:GLU:HB3    | 2.20                     | 0.41              |
| 7:AG:59:LEU:HD23   | 7:AG:60:LYS:N       | 2.35                     | 0.41              |
| 9:AI:106:ALA:O     | 9:AI:108:VAL:N      | 2.52                     | 0.41              |
| 9:AI:91:ASP:C      | 9:AI:93:ARG:N       | 2.69                     | 0.41              |
| 11:AK:107:SER:OG   | 18:AR:86:VAL:HG13   | 2.19                     | 0.41              |
| 12:AL:114:ARG:NH2  | 12:AL:121:LYS:HD3   | 2.32                     | 0.41              |
| 20:AT:89:ARG:CZ    | 20:AT:104:LEU:HD11  | 2.50                     | 0.41              |
| 20:AT:13:LEU:CD1   | 20:AT:17:ARG:HH21   | 2.33                     | 0.41              |
| 24:AX:19:G:H5'     | 24:AX:20:U:C5       | 2.56                     | 0.41              |
| 24:AX:72:A:C6      | 24:AX:73:A:C6       | 3.08                     | 0.41              |
| 56:B7:20:ALA:O     | 56:B7:21:ARG:C      | 2.58                     | 0.41              |
| 58:B9:28:GLU:HB3   | 58:B9:29:ASN:H      | 1.70                     | 0.41              |
| 27:BA:1222:C:H2'   | 27:BA:1223:G:H8     | 1.84                     | 0.41              |
| 27:BA:1278:A:C2    | 27:BA:1279:G:C4     | 3.08                     | 0.41              |
| 27:BA:1419:A:HO2'  | 27:BA:1420:U:H6     | 1.68                     | 0.41              |
| 27:BA:1655:A:H3'   | 27:BA:1656:C:H6     | 1.85                     | 0.41              |
| 27:BA:1714:G:H8    | 27:BA:1714:G:O5'    | 2.02                     | 0.41              |
| 27:BA:2126:A:OP2   | 27:BA:2126:A:H8     | 2.03                     | 0.41              |
| 27:BA:2299:G:C6    | 27:BA:2318:G:C8     | 3.07                     | 0.41              |
| 27:BA:2404:C:O2    | 38:BP:67:MET:HE1    | 2.19                     | 0.41              |
| 27:BA:2524:G:C5'   | 27:BA:2525:G:OP2    | 2.57                     | 0.41              |
| 27:BA:271(M):G:O2' | 27:BA:271(N):U:H5'' | 2.19                     | 0.41              |
| 27:BA:2864:G:H5'   | 27:BA:2864:G:H8     | 1.84                     | 0.41              |
| 27:BA:429:A:C6     | 27:BA:430:G:N1      | 2.88                     | 0.41              |
| 27:BA:497:A:N6     | 27:BA:498:G:C6      | 2.88                     | 0.41              |
| 27:BA:794:G:C5     | 27:BA:795:C:C4      | 3.07                     | 0.41              |
| 27:BA:932:G:H4'    | 27:BA:933:A:O5'     | 2.20                     | 0.41              |
| 29:BC:128:GLY:C    | 29:BC:130:ILE:H     | 2.22                     | 0.41              |
| 30:BD:176:ARG:HA   | 30:BD:182:LEU:HD23  | 2.02                     | 0.41              |
| 30:BD:183:ARG:CG   | 30:BD:183:ARG:HH11  | 2.33                     | 0.41              |
| 30:BD:186:HIS:CD2  | 30:BD:188:GLU:N     | 2.59                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BE:181:LEU:HD21 | 42:BT:7:ILE:HD12  | 2.02                     | 0.41              |
| 31:BE:59:VAL:HG21  | 31:BE:63:LEU:CG   | 2.44                     | 0.41              |
| 31:BE:46:ALA:HB1   | 31:BE:82:ARG:N    | 2.34                     | 0.41              |
| 32:BF:158:THR:C    | 32:BF:178:PRO:HD3 | 2.40                     | 0.41              |
| 32:BF:80:ALA:O     | 32:BF:86:GLY:HA3  | 2.20                     | 0.41              |
| 35:BI:9:LEU:HB2    | 35:BI:12:LEU:O    | 2.20                     | 0.41              |
| 35:BI:51:ILE:O     | 35:BI:55:ALA:HB2  | 2.20                     | 0.41              |
| 35:BI:77:LEU:HD22  | 35:BI:78:THR:H    | 1.81                     | 0.41              |
| 36:BN:3:THR:HA     | 36:BN:4:TYR:CE1   | 2.54                     | 0.41              |
| 38:BP:35:HIS:O     | 38:BP:36:LYS:HB2  | 2.20                     | 0.41              |
| 38:BP:7:ARG:O      | 38:BP:7:ARG:HD3   | 2.20                     | 0.41              |
| 38:BP:9:ASN:H      | 38:BP:10:PRO:HD2  | 1.85                     | 0.41              |
| 41:BS:75:GLU:C     | 41:BS:77:ALA:N    | 2.73                     | 0.41              |
| 41:BS:89:ARG:O     | 41:BS:90:GLY:O    | 2.38                     | 0.41              |
| 42:BT:111:ARG:HE   | 42:BT:111:ARG:HB3 | 1.69                     | 0.41              |
| 42:BT:113:LYS:HA   | 42:BT:113:LYS:HD2 | 1.78                     | 0.41              |
| 42:BT:129:ARG:O    | 42:BT:129:ARG:CG  | 2.64                     | 0.41              |
| 31:BE:52:LEU:CG    | 42:BT:1:MET:HE1   | 2.49                     | 0.41              |
| 42:BT:38:ASN:O     | 42:BT:39:ARG:C    | 2.59                     | 0.41              |
| 27:BA:2848:G:H3'   | 42:BT:95:ARG:O    | 2.20                     | 0.41              |
| 43:BU:8:VAL:HG11   | 43:BU:12:ARG:CZ   | 2.49                     | 0.41              |
| 43:BU:95:LEU:HD13  | 44:BV:4:ILE:HG23  | 2.01                     | 0.41              |
| 47:BY:19:LYS:NZ    | 47:BY:19:LYS:HB2  | 2.35                     | 0.41              |
| 47:BY:14:LEU:N     | 47:BY:73:ARG:O    | 2.53                     | 0.41              |
| 48:BZ:21:GLY:O     | 48:BZ:40:LEU:HB2  | 2.20                     | 0.41              |
| 1:CA:1219:U:H2'    | 1:CA:1220:G:C8    | 2.55                     | 0.41              |
| 1:CA:1286:A:C2     | 21:CU:18:TYR:OH   | 2.71                     | 0.41              |
| 1:CA:1349:A:OP1    | 9:CI:118:LYS:O    | 2.38                     | 0.41              |
| 1:CA:1435:G:H2'    | 1:CA:1436:U:H6    | 1.85                     | 0.41              |
| 1:CA:284:G:C4      | 1:CA:285:G:C8     | 3.07                     | 0.41              |
| 1:CA:322:C:O5'     | 1:CA:322:C:H6     | 2.03                     | 0.41              |
| 1:CA:419:C:C3'     | 1:CA:420:U:H5'    | 2.50                     | 0.41              |
| 1:CA:495:A:H4'     | 1:CA:496:A:O5'    | 2.20                     | 0.41              |
| 1:CA:512:U:H2'     | 1:CA:513:C:C6     | 2.55                     | 0.41              |
| 1:CA:515:G:H2'     | 1:CA:516:U:O4'    | 2.19                     | 0.41              |
| 1:CA:645:C:H2'     | 1:CA:646:U:C6     | 2.53                     | 0.41              |
| 1:CA:732:C:H3'     | 1:CA:732:C:C6     | 2.55                     | 0.41              |
| 1:CA:818:G:C3'     | 1:CA:819:A:C5'    | 2.98                     | 0.41              |
| 1:CA:864:A:H2'     | 1:CA:865:A:O4'    | 2.20                     | 0.41              |
| 1:CA:925:G:H1'     | 1:CA:1502:A:N9    | 2.35                     | 0.41              |
| 2:CB:55:PHE:O      | 2:CB:59:GLU:HB3   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:106:TYR:CG    | 4:CD:114:ARG:HG2   | 2.54                     | 0.41              |
| 4:CD:14:ARG:C      | 4:CD:16:GLY:N      | 2.73                     | 0.41              |
| 5:CE:11:ILE:HD11   | 5:CE:33:VAL:CG2    | 2.50                     | 0.41              |
| 8:CH:13:ILE:N      | 8:CH:13:ILE:HD12   | 2.35                     | 0.41              |
| 8:CH:38:ILE:HD12   | 8:CH:111:ILE:HG23  | 2.02                     | 0.41              |
| 9:CI:40:LEU:HD23   | 9:CI:40:LEU:N      | 2.35                     | 0.41              |
| 12:CL:14:LYS:O     | 12:CL:15:VAL:C     | 2.58                     | 0.41              |
| 12:CL:61:TYR:HB3   | 12:CL:62:GLU:H     | 1.50                     | 0.41              |
| 13:CM:69:GLU:OE1   | 13:CM:72:ALA:N     | 2.53                     | 0.41              |
| 16:CP:48:TRP:CD1   | 16:CP:48:TRP:N     | 2.85                     | 0.41              |
| 12:CL:45:PRO:HB3   | 22:CV:9:G:H4'      | 2.00                     | 0.41              |
| 24:CX:10:G:C2      | 24:CX:26:G:H1'     | 2.54                     | 0.41              |
| 25:CY:46:U:O2'     | 25:CY:47:C:OP1     | 2.33                     | 0.41              |
| 27:DA:1016:G:N1    | 27:DA:1017:G:C5    | 2.88                     | 0.41              |
| 27:DA:1131:G:O2'   | 27:DA:1132:A:H8    | 2.00                     | 0.41              |
| 27:DA:1336:A:O2'   | 27:DA:1337:G:H5'   | 2.19                     | 0.41              |
| 27:DA:1387:C:H2'   | 27:DA:1388:G:C8    | 2.51                     | 0.41              |
| 27:DA:141:A:H8     | 27:DA:1408:C:HO2'  | 1.51                     | 0.41              |
| 27:DA:143(A):C:O2' | 27:DA:144:C:H5'    | 2.20                     | 0.41              |
| 27:DA:1677:A:H2'   | 27:DA:1678:G:C8    | 2.54                     | 0.41              |
| 27:DA:2171:A:C4'   | 27:DA:2172:U:OP1   | 2.68                     | 0.41              |
| 27:DA:221:A:N7     | 27:DA:266:G:O6     | 2.53                     | 0.41              |
| 27:DA:2355:C:H4'   | 49:D0:24:LYS:CG    | 2.47                     | 0.41              |
| 27:DA:241:A:O4'    | 27:DA:243:U:C6     | 2.73                     | 0.41              |
| 27:DA:2428:G:H4'   | 27:DA:2429:G:N7    | 2.35                     | 0.41              |
| 27:DA:957:A:N1     | 27:DA:2459:A:H8    | 2.18                     | 0.41              |
| 27:DA:2465:C:O2'   | 27:DA:2466:C:H5'   | 2.20                     | 0.41              |
| 27:DA:2591:C:P     | 30:DD:239:ARG:HB3  | 2.60                     | 0.41              |
| 27:DA:2648:C:H2'   | 27:DA:2649:U:H6    | 1.81                     | 0.41              |
| 27:DA:2772:C:H6    | 27:DA:2772:C:O5'   | 2.03                     | 0.41              |
| 27:DA:2784:C:O2    | 31:DE:37:ARG:NH2   | 2.52                     | 0.41              |
| 27:DA:2790:A:O2'   | 27:DA:2893:G:N3    | 2.46                     | 0.41              |
| 27:DA:321:G:C2     | 27:DA:341:G:H4'    | 2.55                     | 0.41              |
| 27:DA:359:A:H2'    | 27:DA:360:G:O4'    | 2.20                     | 0.41              |
| 27:DA:363(A):A:N3  | 27:DA:363(A):A:H2' | 2.34                     | 0.41              |
| 27:DA:782:A:H5'    | 27:DA:783:A:C2     | 2.55                     | 0.41              |
| 27:DA:888:C:H2'    | 27:DA:889:C:H5'    | 2.02                     | 0.41              |
| 27:DA:888:C:H3'    | 27:DA:889:C:C5'    | 2.50                     | 0.41              |
| 28:DB:92:C:O2'     | 28:DB:93:G:H5'     | 2.20                     | 0.41              |
| 30:DD:8:PRO:O      | 30:DD:10:THR:N     | 2.53                     | 0.41              |
| 32:DF:114:VAL:HG21 | 32:DF:202:PHE:CZ   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 33:DG:131:TYR:O   | 33:DG:159:VAL:HG13  | 2.20                     | 0.41              |
| 33:DG:170:ARG:O   | 33:DG:170:ARG:HD2   | 2.19                     | 0.41              |
| 33:DG:14:GLU:O    | 33:DG:17:PRO:HG2    | 2.20                     | 0.41              |
| 33:DG:64:THR:HG23 | 33:DG:66:GLN:N      | 2.34                     | 0.41              |
| 33:DG:77:ILE:HG22 | 33:DG:80:PHE:H      | 1.85                     | 0.41              |
| 35:DI:68:LEU:HA   | 35:DI:71:ILE:HG12   | 2.02                     | 0.41              |
| 36:DN:136:GLU:OE1 | 36:DN:137:LYS:N     | 2.50                     | 0.41              |
| 36:DN:54:VAL:HG12 | 36:DN:54:VAL:O      | 2.19                     | 0.41              |
| 27:DA:1278:A:C5'  | 40:DR:36:THR:HG22   | 2.44                     | 0.41              |
| 40:DR:47:PHE:C    | 40:DR:47:PHE:CD2    | 2.94                     | 0.41              |
| 43:DU:74:LEU:HD21 | 43:DU:110:VAL:HG13  | 2.02                     | 0.41              |
| 27:DA:974:G:OP1   | 44:DV:76:LYS:HE3    | 2.19                     | 0.41              |
| 45:DW:12:ILE:HG13 | 45:DW:42:ARG:HH12   | 1.84                     | 0.41              |
| 46:DX:13:LEU:HA   | 46:DX:13:LEU:HD23   | 1.88                     | 0.41              |
| 47:DY:95:LYS:HD3  | 47:DY:100:ALA:HA    | 2.02                     | 0.41              |
| 47:DY:54:LYS:NZ   | 47:DY:55:TYR:HE2    | 2.18                     | 0.41              |
| 47:DY:96:ILE:CG2  | 47:DY:97:ARG:H      | 2.30                     | 0.41              |
| 48:DZ:18:ARG:HA   | 48:DZ:22:LYS:O      | 2.20                     | 0.41              |
| 1:AA:1172:C:H2'   | 1:AA:1173:G:H8      | 1.82                     | 0.41              |
| 1:AA:1233:G:H2'   | 1:AA:1234:C:H6      | 1.80                     | 0.41              |
| 1:AA:1314:C:OP2   | 19:AS:6:LYS:HD3     | 2.20                     | 0.41              |
| 1:AA:1442:G:H2'   | 1:AA:1442(A):G:H5'' | 2.01                     | 0.41              |
| 1:AA:381:C:H2'    | 1:AA:382:A:O4'      | 2.20                     | 0.41              |
| 1:AA:528:C:H5'    | 1:AA:535:A:C6       | 2.54                     | 0.41              |
| 1:AA:637:G:C2'    | 1:AA:638:G:H5'      | 2.50                     | 0.41              |
| 1:AA:728:A:C5     | 15:AO:54:ARG:CD     | 3.04                     | 0.41              |
| 1:AA:740:U:OP2    | 15:AO:2:PRO:HG3     | 2.20                     | 0.41              |
| 1:AA:661:G:H1     | 1:AA:744:C:H42      | 1.66                     | 0.41              |
| 1:AA:914:A:H2'    | 1:AA:915:A:H8       | 1.85                     | 0.41              |
| 2:AB:207:ALA:O    | 2:AB:209:ARG:N      | 2.54                     | 0.41              |
| 2:AB:95:GLN:O     | 2:AB:97:TRP:N       | 2.53                     | 0.41              |
| 3:AC:33:LEU:O     | 3:AC:36:ASP:HB2     | 2.20                     | 0.41              |
| 4:AD:122:ARG:HD3  | 4:AD:122:ARG:O      | 2.20                     | 0.41              |
| 4:AD:163:GLU:C    | 4:AD:165:MET:H      | 2.23                     | 0.41              |
| 4:AD:33:MET:HE3   | 4:AD:33:MET:HA      | 2.02                     | 0.41              |
| 4:AD:94:LEU:HA    | 4:AD:97:LEU:HD12    | 2.01                     | 0.41              |
| 10:AJ:7:LYS:CD    | 10:AJ:71:LEU:HD13   | 2.50                     | 0.41              |
| 10:AJ:84:GLN:C    | 10:AJ:85:LEU:HD23   | 2.41                     | 0.41              |
| 1:AA:36:C:C4'     | 12:AL:119:THR:O     | 2.68                     | 0.41              |
| 12:AL:24:LEU:C    | 12:AL:26:GLY:H      | 2.23                     | 0.41              |
| 14:AN:58:LYS:O    | 14:AN:59:ALA:O      | 2.38                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:AR:62:GLU:O     | 18:AR:65:ILE:N     | 2.53                     | 0.41              |
| 19:AS:15:LEU:HD13  | 19:AS:15:LEU:HA    | 1.87                     | 0.41              |
| 21:AU:24:ARG:O     | 21:AU:25:LYS:CB    | 2.68                     | 0.41              |
| 23:AW:10:G:C2      | 23:AW:25:A:H1'     | 2.54                     | 0.41              |
| 25:AY:11:C:H2'     | 25:AY:12:C:C6      | 2.55                     | 0.41              |
| 50:B1:6:GLU:HG3    | 50:B1:61:ARG:O     | 2.19                     | 0.41              |
| 51:B2:42:GLY:O     | 51:B2:43:GLN:C     | 2.58                     | 0.41              |
| 51:B2:9:GLN:NE2    | 51:B2:56:GLN:CD    | 2.73                     | 0.41              |
| 51:B2:59:ARG:O     | 51:B2:62:THR:HB    | 2.20                     | 0.41              |
| 58:B9:29:ASN:ND2   | 58:B9:32:HIS:ND1   | 2.64                     | 0.41              |
| 27:BA:1307:A:C2    | 27:BA:1308:A:C4    | 3.08                     | 0.41              |
| 27:BA:1308:A:H2'   | 27:BA:1309:G:O4'   | 2.20                     | 0.41              |
| 27:BA:1417:C:H2'   | 27:BA:1418:G:O4'   | 2.19                     | 0.41              |
| 27:BA:1509(B):A:C4 | 27:BA:1510:G:C8    | 3.08                     | 0.41              |
| 27:BA:1668:A:N7    | 27:BA:1674:G:C5    | 2.88                     | 0.41              |
| 27:BA:1722:A:C6    | 27:BA:1741:A:N1    | 2.89                     | 0.41              |
| 27:BA:1836:C:H2'   | 27:BA:1837:C:H5'   | 2.01                     | 0.41              |
| 27:BA:528:A:C2     | 27:BA:2043:C:H4'   | 2.55                     | 0.41              |
| 27:BA:211:A:H2'    | 27:BA:212:G:C8     | 2.54                     | 0.41              |
| 27:BA:2240:C:C2    | 27:BA:2241:A:C8    | 3.08                     | 0.41              |
| 27:BA:2446:G:C2    | 27:BA:2501:C:C5    | 3.09                     | 0.41              |
| 27:BA:2694:G:C6    | 27:BA:2695:C:C4    | 3.09                     | 0.41              |
| 27:BA:2809:A:N3    | 27:BA:2892:A:N3    | 2.68                     | 0.41              |
| 27:BA:299:A:H62    | 27:BA:300:A:N6     | 2.18                     | 0.41              |
| 27:BA:846:C:C1'    | 27:BA:847:U:C5     | 3.03                     | 0.41              |
| 28:BB:7:G:H3'      | 28:BB:8:U:C5'      | 2.41                     | 0.41              |
| 29:BC:76:ALA:O     | 29:BC:78:ALA:N     | 2.53                     | 0.41              |
| 30:BD:133:LEU:HD13 | 30:BD:173:VAL:HG11 | 2.01                     | 0.41              |
| 30:BD:228:PRO:O    | 30:BD:229:VAL:C    | 2.58                     | 0.41              |
| 27:BA:1656:C:H5''  | 31:BE:136:ARG:HB2  | 2.02                     | 0.41              |
| 32:BF:140:LEU:HD21 | 32:BF:170:LEU:HD11 | 2.02                     | 0.41              |
| 32:BF:152:GLU:O    | 32:BF:154:VAL:HG23 | 2.20                     | 0.41              |
| 32:BF:188:ARG:HB2  | 38:BP:7:ARG:NH2    | 2.34                     | 0.41              |
| 32:BF:184:TYR:HE2  | 32:BF:188:ARG:HD2  | 1.82                     | 0.41              |
| 32:BF:77:ASP:N     | 32:BF:77:ASP:OD1   | 2.52                     | 0.41              |
| 33:BG:99:MET:O     | 33:BG:102:PHE:HB3  | 2.19                     | 0.41              |
| 34:BH:106:THR:O    | 34:BH:106:THR:OG1  | 2.34                     | 0.41              |
| 34:BH:137:ASP:HB3  | 34:BH:138:LYS:H    | 1.63                     | 0.41              |
| 35:BI:81:VAL:HG12  | 35:BI:82:ARG:H     | 1.85                     | 0.41              |
| 27:BA:1246:A:P     | 38:BP:18:ARG:HG3   | 2.59                     | 0.41              |
| 27:BA:631:A:OP1    | 38:BP:64:LYS:HE3   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:BQ:12:GLN:HE21 | 39:BQ:73:PRO:HD3  | 1.85                     | 0.41              |
| 39:BQ:43:THR:OG1  | 39:BQ:46:GLN:HG3  | 2.20                     | 0.41              |
| 39:BQ:56:ARG:CG   | 39:BQ:56:ARG:NH1  | 2.82                     | 0.41              |
| 40:BR:109:ALA:O   | 40:BR:111:LEU:CD2 | 2.69                     | 0.41              |
| 42:BT:20:PRO:HG2  | 42:BT:85:LYS:O    | 2.20                     | 0.41              |
| 42:BT:30:VAL:HG12 | 42:BT:44:ASP:OD2  | 2.20                     | 0.41              |
| 44:BV:62:LEU:HD23 | 44:BV:93:GLU:CB   | 2.48                     | 0.41              |
| 44:BV:91:TYR:C    | 44:BV:92:THR:CG2  | 2.89                     | 0.41              |
| 45:BW:92:ARG:HH11 | 45:BW:92:ARG:HB3  | 1.84                     | 0.41              |
| 46:BX:34:ALA:O    | 46:BX:35:THR:HG23 | 2.19                     | 0.41              |
| 46:BX:63:LYS:HA   | 46:BX:72:LYS:HA   | 2.02                     | 0.41              |
| 48:BZ:2:TYR:O     | 48:BZ:3:ARG:HB2   | 2.19                     | 0.41              |
| 1:CA:1014:A:C5    | 1:CA:1015:A:C6    | 3.08                     | 0.41              |
| 1:CA:1043:C:H2'   | 1:CA:1044:A:C8    | 2.54                     | 0.41              |
| 1:CA:1102:A:C6    | 1:CA:1103:C:N4    | 2.87                     | 0.41              |
| 1:CA:1222:G:H2'   | 1:CA:1223:C:O4'   | 2.19                     | 0.41              |
| 1:CA:926:G:C6     | 1:CA:1505:G:C6    | 3.08                     | 0.41              |
| 1:CA:172:A:N7     | 1:CA:174:C:C4     | 2.88                     | 0.41              |
| 1:CA:221:C:HO2'   | 1:CA:222:U:H5'    | 1.84                     | 0.41              |
| 1:CA:312:C:H2'    | 1:CA:313:A:C8     | 2.55                     | 0.41              |
| 1:CA:653:A:C4'    | 8:CH:56:LYS:HZ3   | 2.32                     | 0.41              |
| 1:CA:701:C:O2'    | 1:CA:703:G:C5     | 2.71                     | 0.41              |
| 1:CA:923:A:C6     | 1:CA:924:C:C4     | 3.09                     | 0.41              |
| 1:CA:938:A:N6     | 1:CA:939:G:C6     | 2.89                     | 0.41              |
| 1:CA:968:A:H4'    | 1:CA:969:A:OP2    | 2.20                     | 0.41              |
| 2:CB:153:ARG:HG3  | 2:CB:153:ARG:H    | 1.49                     | 0.41              |
| 4:CD:113:SER:O    | 4:CD:116:GLN:N    | 2.53                     | 0.41              |
| 4:CD:96:LEU:HG    | 4:CD:139:ARG:NH1  | 2.35                     | 0.41              |
| 5:CE:101:ILE:HD11 | 5:CE:118:ILE:O    | 2.21                     | 0.41              |
| 5:CE:45:PHE:C     | 5:CE:45:PHE:HD1   | 2.22                     | 0.41              |
| 6:CF:1:MET:HB3    | 6:CF:66:GLU:OE2   | 2.19                     | 0.41              |
| 10:CJ:38:ILE:HA   | 10:CJ:39:PRO:HD3  | 1.82                     | 0.41              |
| 10:CJ:6:ILE:O     | 10:CJ:71:LEU:HD12 | 2.19                     | 0.41              |
| 10:CJ:30:SER:CA   | 10:CJ:80:LYS:HD3  | 2.50                     | 0.41              |
| 12:CL:112:LYS:O   | 12:CL:114:ARG:HG3 | 2.20                     | 0.41              |
| 13:CM:90:LEU:O    | 13:CM:91:ARG:CG   | 2.68                     | 0.41              |
| 1:CA:1186:G:N2    | 14:CN:61:TRP:C    | 2.73                     | 0.41              |
| 20:CT:54:LYS:HB2  | 20:CT:54:LYS:HE3  | 1.79                     | 0.41              |
| 24:CX:52:G:H2'    | 24:CX:53:G:H8     | 1.85                     | 0.41              |
| 49:D0:41:ARG:CD   | 49:D0:41:ARG:N    | 2.66                     | 0.41              |
| 49:D0:72:ARG:HB3  | 49:D0:75:LEU:HB3  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:D0:45:PHE:CZ   | 49:D0:77:ARG:NH1   | 2.88                     | 0.41              |
| 51:D2:10:LEU:O    | 51:D2:14:ARG:CG    | 2.68                     | 0.41              |
| 52:D3:19:GLN:NE2  | 52:D3:52:HIS:CE1   | 2.88                     | 0.41              |
| 52:D3:56:VAL:HG12 | 52:D3:57:GLU:N     | 2.35                     | 0.41              |
| 27:DA:2611:U:C6   | 54:D5:4:HIS:HE1    | 2.38                     | 0.41              |
| 56:D7:41:ARG:N    | 56:D7:41:ARG:NH1   | 2.68                     | 0.41              |
| 57:D8:40:GLU:O    | 57:D8:41:ILE:C     | 2.58                     | 0.41              |
| 58:D9:17:ILE:O    | 58:D9:24:TYR:N     | 2.40                     | 0.41              |
| 27:DA:1151:G:C6   | 27:DA:1152:C:C4    | 3.07                     | 0.41              |
| 27:DA:1208:C:H2'  | 27:DA:1209:G:H5'   | 2.01                     | 0.41              |
| 27:DA:1680:U:H2'  | 27:DA:1681:G:O4'   | 2.20                     | 0.41              |
| 27:DA:1764:G:N2   | 27:DA:1765:C:C1'   | 2.83                     | 0.41              |
| 27:DA:1859:A:N6   | 27:DA:1860:G:C2    | 2.88                     | 0.41              |
| 27:DA:1866:C:H2'  | 27:DA:1876:A:O4'   | 2.19                     | 0.41              |
| 27:DA:1933:G:H2'  | 27:DA:1934:C:H6    | 1.82                     | 0.41              |
| 27:DA:2306:C:H5   | 27:DA:2307:G:O2'   | 2.02                     | 0.41              |
| 27:DA:241:A:H2    | 27:DA:242:G:N2     | 2.18                     | 0.41              |
| 27:DA:2581:G:H22  | 27:DA:2610:C:H2'   | 1.85                     | 0.41              |
| 27:DA:2635:C:H4'  | 31:DE:78:LEU:O     | 2.20                     | 0.41              |
| 27:DA:2645:G:H3'  | 27:DA:2646:C:C5'   | 2.50                     | 0.41              |
| 27:DA:2848:G:C2   | 27:DA:2867:G:C4    | 3.08                     | 0.41              |
| 27:DA:371:A:O3'   | 27:DA:372:G:H4'    | 2.20                     | 0.41              |
| 27:DA:397:G:C6    | 27:DA:398:G:N7     | 2.88                     | 0.41              |
| 27:DA:479:A:H4'   | 27:DA:480:A:O5'    | 2.20                     | 0.41              |
| 27:DA:573:G:O2'   | 27:DA:574:C:H3'    | 2.20                     | 0.41              |
| 27:DA:588:U:C2    | 32:DF:90:PHE:CD1   | 3.08                     | 0.41              |
| 27:DA:634:C:O2'   | 27:DA:635:C:C6     | 2.70                     | 0.41              |
| 27:DA:918:A:H3'   | 27:DA:919:G:C8     | 2.49                     | 0.41              |
| 27:DA:959:A:O2'   | 27:DA:960:A:H5'    | 2.20                     | 0.41              |
| 30:DD:76:PRO:HG2  | 30:DD:98:VAL:HG21  | 2.02                     | 0.41              |
| 33:DG:119:GLY:O   | 33:DG:181:ARG:CZ   | 2.69                     | 0.41              |
| 33:DG:51:ARG:NH1  | 33:DG:53:LEU:HD21  | 2.35                     | 0.41              |
| 33:DG:64:THR:CG2  | 33:DG:65:GLY:N     | 2.83                     | 0.41              |
| 36:DN:15:LEU:HD22 | 36:DN:16:ILE:N     | 2.28                     | 0.41              |
| 37:DO:107:ARG:NH1 | 42:DT:36:GLU:H     | 2.18                     | 0.41              |
| 37:DO:73:ASP:C    | 37:DO:73:ASP:OD1   | 2.58                     | 0.41              |
| 38:DP:87:ASP:N    | 38:DP:87:ASP:OD1   | 2.53                     | 0.41              |
| 40:DR:111:LEU:HA  | 40:DR:111:LEU:HD13 | 1.84                     | 0.41              |
| 41:DS:17:ARG:O    | 41:DS:18:ILE:CB    | 2.48                     | 0.41              |
| 43:DU:60:LEU:HA   | 43:DU:60:LEU:HD22  | 1.64                     | 0.41              |
| 47:DY:88:LYS:HB3  | 47:DY:90:LEU:HD12  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1026:G:C3'   | 1:AA:1027:C:H5'   | 2.48                     | 0.41              |
| 1:AA:1074:G:H1    | 1:AA:1083:U:H3    | 1.68                     | 0.41              |
| 1:AA:1278:U:H3'   | 1:AA:1278:U:H6    | 1.84                     | 0.41              |
| 1:AA:1486:G:H2'   | 1:AA:1487:G:C1'   | 2.50                     | 0.41              |
| 1:AA:261:U:H3'    | 1:AA:263:A:OP2    | 2.20                     | 0.41              |
| 1:AA:279:A:O5'    | 1:AA:281:G:H5'    | 2.20                     | 0.41              |
| 1:AA:492:G:C5     | 1:AA:493:G:C8     | 3.09                     | 0.41              |
| 1:AA:573:A:C6     | 1:AA:574:A:N1     | 2.88                     | 0.41              |
| 1:AA:61:G:C6      | 1:AA:62:U:O4      | 2.73                     | 0.41              |
| 1:AA:690:G:H2'    | 1:AA:691:G:O4'    | 2.20                     | 0.41              |
| 1:AA:782:A:N1     | 1:AA:801:U:C2     | 2.88                     | 0.41              |
| 1:AA:825:G:C6     | 1:AA:876:G:C6     | 3.09                     | 0.41              |
| 1:AA:900:A:H2'    | 1:AA:901:A:O4'    | 2.20                     | 0.41              |
| 2:AB:15:VAL:H     | 2:AB:16:HIS:CE1   | 2.39                     | 0.41              |
| 4:AD:162:LEU:HD12 | 4:AD:181:MET:SD   | 2.61                     | 0.41              |
| 5:AE:56:GLN:O     | 5:AE:57:LYS:C     | 2.58                     | 0.41              |
| 7:AG:108:ALA:C    | 7:AG:110:GLN:N    | 2.74                     | 0.41              |
| 7:AG:120:ILE:HG22 | 7:AG:124:LEU:HD11 | 2.02                     | 0.41              |
| 7:AG:50:ILE:O     | 7:AG:54:THR:CG2   | 2.68                     | 0.41              |
| 7:AG:71:PRO:HG3   | 7:AG:99:LEU:HD12  | 2.02                     | 0.41              |
| 7:AG:72:ARG:HA    | 7:AG:72:ARG:HD2   | 1.93                     | 0.41              |
| 8:AH:105:ARG:HD3  | 8:AH:105:ARG:HA   | 1.70                     | 0.41              |
| 8:AH:100:ILE:CB   | 8:AH:125:ARG:HH12 | 2.32                     | 0.41              |
| 8:AH:1:MET:SD     | 8:AH:2:LEU:N      | 2.92                     | 0.41              |
| 10:AJ:32:ALA:HB3  | 10:AJ:75:ILE:HD11 | 2.02                     | 0.41              |
| 10:AJ:40:LEU:HD23 | 10:AJ:40:LEU:H    | 1.83                     | 0.41              |
| 10:AJ:58:ASP:O    | 10:AJ:59:SER:C    | 2.58                     | 0.41              |
| 13:AM:5:ALA:HB1   | 13:AM:66:LEU:HD22 | 2.01                     | 0.41              |
| 13:AM:65:LYS:CB   | 13:AM:70:LEU:HB2  | 2.49                     | 0.41              |
| 20:AT:13:LEU:HD12 | 20:AT:14:LYS:N    | 2.35                     | 0.41              |
| 20:AT:24:LEU:O    | 20:AT:25:ARG:C    | 2.58                     | 0.41              |
| 23:AW:30:A:H3'    | 23:AW:31:U:H5''   | 2.01                     | 0.41              |
| 52:B3:22:ALA:HA   | 52:B3:46:ASN:HD22 | 1.85                     | 0.41              |
| 56:B7:45:ALA:O    | 56:B7:46:VAL:HG23 | 2.18                     | 0.41              |
| 58:B9:2:LYS:C     | 58:B9:2:LYS:HD3   | 2.40                     | 0.41              |
| 27:BA:1139:G:C2'  | 27:BA:1140:C:O5'  | 2.68                     | 0.41              |
| 27:BA:1452:A:O2'  | 27:BA:1453:U:H6   | 2.03                     | 0.41              |
| 27:BA:1624:G:N2   | 27:BA:1625:C:H1'  | 2.35                     | 0.41              |
| 27:BA:1627:G:O2'  | 27:BA:1628:G:H5'  | 2.21                     | 0.41              |
| 27:BA:1762:A:H8   | 27:BA:1762:A:P    | 2.43                     | 0.41              |
| 27:BA:1815:A:H4'  | 27:BA:1816:G:OP1  | 2.18                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1926:U:O2   | 27:BA:1928:A:C8    | 2.73                     | 0.41              |
| 27:BA:2027:G:C2'  | 27:BA:2028:U:H5'   | 2.50                     | 0.41              |
| 27:BA:2223:G:C2'  | 27:BA:2224:G:H5'   | 2.49                     | 0.41              |
| 27:BA:272(H):C:O2 | 27:BA:272(H):C:H2' | 2.20                     | 0.41              |
| 27:BA:2791:C:H5'  | 27:BA:2792:G:OP1   | 2.20                     | 0.41              |
| 27:BA:2844:G:H2'  | 27:BA:2845:G:H5'   | 2.02                     | 0.41              |
| 27:BA:2846:G:H2'  | 27:BA:2847:U:O4'   | 2.20                     | 0.41              |
| 27:BA:2848:G:HO2' | 27:BA:2867:G:H22   | 1.68                     | 0.41              |
| 27:BA:452:G:C6    | 27:BA:453:C:C5     | 3.08                     | 0.41              |
| 27:BA:459:U:C2    | 27:BA:460:A:C8     | 3.08                     | 0.41              |
| 27:BA:482:A:H5''  | 47:BY:47:LYS:HG2   | 2.03                     | 0.41              |
| 27:BA:495:G:O2'   | 45:BW:62:HIS:HE1   | 2.03                     | 0.41              |
| 27:BA:51:G:H4'    | 27:BA:52:A:H5'     | 2.02                     | 0.41              |
| 27:BA:533:G:H2'   | 27:BA:534:U:O4'    | 2.21                     | 0.41              |
| 27:BA:620:G:C4'   | 27:BA:621:A:OP1    | 2.68                     | 0.41              |
| 27:BA:81:G:C2     | 27:BA:106:C:C2     | 3.08                     | 0.41              |
| 27:BA:861:A:C6    | 27:BA:917:A:C8     | 3.08                     | 0.41              |
| 27:BA:840:C:C2    | 27:BA:939:G:N1     | 2.88                     | 0.41              |
| 30:BD:24:ILE:HD12 | 30:BD:27:THR:HG23  | 2.02                     | 0.41              |
| 30:BD:69:ARG:NH2  | 30:BD:128:GLY:O    | 2.53                     | 0.41              |
| 33:BG:11:TYR:O    | 33:BG:16:ARG:HB2   | 2.20                     | 0.41              |
| 34:BH:148:ILE:HA  | 34:BH:148:ILE:HD13 | 1.90                     | 0.41              |
| 34:BH:169:VAL:O   | 34:BH:169:VAL:HG13 | 2.20                     | 0.41              |
| 34:BH:55:PRO:HG2  | 34:BH:61:HIS:CE1   | 2.54                     | 0.41              |
| 35:BI:11:ASN:HB3  | 35:BI:12:LEU:CD2   | 2.51                     | 0.41              |
| 36:BN:27:ALA:O    | 36:BN:28:THR:C     | 2.58                     | 0.41              |
| 39:BQ:67:ARG:HD2  | 39:BQ:105:GLU:OE1  | 2.19                     | 0.41              |
| 41:BS:102:ALA:O   | 41:BS:103:GLU:C    | 2.59                     | 0.41              |
| 42:BT:106:SER:O   | 42:BT:107:ASP:OD1  | 2.39                     | 0.41              |
| 43:BU:31:SER:C    | 43:BU:33:ARG:N     | 2.72                     | 0.41              |
| 45:BW:54:ALA:HB1  | 45:BW:107:LEU:HD22 | 2.01                     | 0.41              |
| 45:BW:68:ARG:HD3  | 45:BW:110:LYS:HB3  | 2.02                     | 0.41              |
| 45:BW:6:ILE:HA    | 45:BW:104:THR:HA   | 2.02                     | 0.41              |
| 47:BY:38:ILE:HA   | 47:BY:38:ILE:HD13  | 1.79                     | 0.41              |
| 47:BY:7:VAL:CA    | 47:BY:8:LYS:HD2    | 2.50                     | 0.41              |
| 1:CA:1229:A:O2'   | 1:CA:1230:C:O4'    | 2.34                     | 0.41              |
| 1:CA:1335:C:H5''  | 1:CA:1336:C:O5'    | 2.21                     | 0.41              |
| 1:CA:1435:G:H2'   | 1:CA:1436:U:C6     | 2.55                     | 0.41              |
| 1:CA:481:G:O2'    | 1:CA:483:C:N4      | 2.53                     | 0.41              |
| 1:CA:59:A:H1'     | 1:CA:354:G:C2      | 2.55                     | 0.41              |
| 1:CA:622:A:C8     | 1:CA:623:C:C6      | 3.07                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:943:U:H1'    | 9:CI:124:GLN:HE22  | 1.85                     | 0.41              |
| 2:CB:177:ALA:HB1  | 2:CB:182:ILE:HB    | 2.02                     | 0.41              |
| 3:CC:84:ILE:HA    | 3:CC:87:LEU:HG     | 2.02                     | 0.41              |
| 3:CC:99:VAL:CG2   | 3:CC:99:VAL:O      | 2.68                     | 0.41              |
| 4:CD:102:ASP:O    | 4:CD:117:ALA:HB1   | 2.19                     | 0.41              |
| 4:CD:121:VAL:HG22 | 4:CD:126:ILE:CG1   | 2.50                     | 0.41              |
| 4:CD:154:ASN:O    | 4:CD:155:LEU:HD23  | 2.20                     | 0.41              |
| 6:CF:10:LEU:N     | 6:CF:10:LEU:CD1    | 2.79                     | 0.41              |
| 8:CH:104:ARG:HD2  | 8:CH:104:ARG:HA    | 1.74                     | 0.41              |
| 8:CH:69:ARG:HD3   | 8:CH:76:PRO:HA     | 2.02                     | 0.41              |
| 9:CI:125:TYR:C    | 9:CI:125:TYR:HD2   | 2.23                     | 0.41              |
| 12:CL:35:THR:CG2  | 12:CL:56:ARG:NH1   | 2.83                     | 0.41              |
| 12:CL:35:THR:HG22 | 12:CL:56:ARG:HH12  | 1.85                     | 0.41              |
| 16:CP:33:ILE:HG21 | 16:CP:59:TRP:CH2   | 2.55                     | 0.41              |
| 16:CP:49:LEU:HG   | 16:CP:49:LEU:O     | 2.20                     | 0.41              |
| 16:CP:57:ARG:O    | 16:CP:58:TYR:C     | 2.58                     | 0.41              |
| 17:CQ:85:VAL:O    | 17:CQ:89:LEU:HB2   | 2.21                     | 0.41              |
| 18:CR:70:ILE:HG22 | 18:CR:71:LYS:N     | 2.34                     | 0.41              |
| 50:D1:25:LYS:HD3  | 50:D1:31:GLY:H     | 1.84                     | 0.41              |
| 51:D2:47:ASN:C    | 51:D2:49:LYS:N     | 2.74                     | 0.41              |
| 53:D4:36:VAL:HG21 | 53:D4:53:THR:HA    | 2.02                     | 0.41              |
| 27:DA:108:U:H2'   | 27:DA:109:G:C8     | 2.51                     | 0.41              |
| 27:DA:1381:G:H1'  | 27:DA:1571:A:N1    | 2.34                     | 0.41              |
| 27:DA:1719:G:O2'  | 27:DA:1720:U:H5'   | 2.19                     | 0.41              |
| 27:DA:1797:C:O2   | 27:DA:1797:C:H2'   | 2.19                     | 0.41              |
| 27:DA:1905:C:N4   | 27:DA:1930:G:N1    | 2.68                     | 0.41              |
| 27:DA:1945:G:O2'  | 27:DA:1946:U:O5'   | 2.38                     | 0.41              |
| 27:DA:2008:C:H2'  | 27:DA:2009:G:H8    | 1.86                     | 0.41              |
| 27:DA:2550:G:N7   | 27:DA:2551:C:C5    | 2.88                     | 0.41              |
| 27:DA:2074:U:H4'  | 27:DA:2598:A:O4'   | 2.20                     | 0.41              |
| 27:DA:2620:C:OP1  | 31:DE:152:LYS:O    | 2.38                     | 0.41              |
| 27:DA:272(E):G:C6 | 27:DA:272(F):C:N3  | 2.88                     | 0.41              |
| 27:DA:2854:G:H2'  | 27:DA:2855:C:C6    | 2.55                     | 0.41              |
| 27:DA:391:G:H1'   | 27:DA:411:G:O4'    | 2.20                     | 0.41              |
| 27:DA:913:U:H6    | 27:DA:913:U:O5'    | 2.04                     | 0.41              |
| 30:DD:123:ALA:HB3 | 30:DD:131:LEU:HD11 | 2.03                     | 0.41              |
| 30:DD:52:ARG:C    | 30:DD:53:PHE:CG    | 2.92                     | 0.41              |
| 30:DD:49:ILE:HD11 | 30:DD:52:ARG:HA    | 2.02                     | 0.41              |
| 32:DF:101:LEU:O   | 32:DF:102:PRO:C    | 2.58                     | 0.41              |
| 32:DF:140:LEU:O   | 32:DF:143:ALA:HB3  | 2.21                     | 0.41              |
| 32:DF:3:GLU:HG2   | 32:DF:4:VAL:H      | 1.84                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DF:63:LYS:HZ2  | 32:DF:67:GLN:HB3   | 1.85                     | 0.41              |
| 34:DH:58:GLU:C    | 34:DH:60:ARG:N     | 2.73                     | 0.41              |
| 35:DI:8:PRO:HA    | 35:DI:14:ASP:H     | 1.84                     | 0.41              |
| 38:DP:9:ASN:ND2   | 38:DP:9:ASN:N      | 2.65                     | 0.41              |
| 40:DR:4:LEU:HD22  | 40:DR:4:LEU:C      | 2.39                     | 0.41              |
| 42:DT:13:ARG:NH1  | 42:DT:15:VAL:HG11  | 2.35                     | 0.41              |
| 42:DT:30:VAL:HG21 | 42:DT:83:ILE:CG1   | 2.50                     | 0.41              |
| 42:DT:61:PHE:O    | 42:DT:61:PHE:CG    | 2.73                     | 0.41              |
| 44:DV:62:LEU:N    | 44:DV:62:LEU:CD2   | 2.81                     | 0.41              |
| 27:DA:1188:U:C4'  | 44:DV:79:VAL:CG2   | 2.92                     | 0.41              |
| 45:DW:7:ALA:CB    | 45:DW:103:ILE:HB   | 2.23                     | 0.41              |
| 45:DW:107:LEU:N   | 45:DW:107:LEU:HD12 | 2.35                     | 0.41              |
| 27:DA:143:G:H1'   | 46:DX:37:THR:HG21  | 1.99                     | 0.41              |
| 46:DX:92:LEU:C    | 46:DX:94:GLY:H     | 2.15                     | 0.41              |
| 47:DY:2:ARG:C     | 47:DY:3:VAL:HG23   | 2.41                     | 0.41              |
| 47:DY:46:LYS:HD3  | 47:DY:47:LYS:HZ2   | 1.84                     | 0.41              |
| 48:DZ:127:VAL:CG2 | 48:DZ:131:ASN:HB2  | 2.50                     | 0.41              |
| 48:DZ:86:ASP:O    | 48:DZ:87:PHE:CD2   | 2.73                     | 0.41              |
| 1:AA:1066:C:O2'   | 1:AA:1067:A:C5'    | 2.68                     | 0.41              |
| 1:AA:1192:C:O2    | 5:AE:25:ARG:NH2    | 2.47                     | 0.41              |
| 1:AA:171:A:N6     | 1:AA:172:A:C6      | 2.89                     | 0.41              |
| 1:AA:472:A:C6     | 1:AA:473:G:N3      | 2.88                     | 0.41              |
| 1:AA:616:G:C2     | 1:AA:617:G:C8      | 3.08                     | 0.41              |
| 1:AA:632:A:C8     | 1:AA:633:G:C8      | 3.08                     | 0.41              |
| 1:AA:680:C:C2     | 1:AA:711:G:N2      | 2.88                     | 0.41              |
| 1:AA:773:G:H1     | 1:AA:806:C:H42     | 1.68                     | 0.41              |
| 1:AA:912:C:O2'    | 1:AA:913:A:H5'     | 2.20                     | 0.41              |
| 2:AB:173:ALA:O    | 2:AB:174:VAL:C     | 2.58                     | 0.41              |
| 2:AB:213:LEU:O    | 2:AB:214:ILE:C     | 2.59                     | 0.41              |
| 3:AC:143:GLU:O    | 3:AC:145:GLY:N     | 2.53                     | 0.41              |
| 3:AC:201:TYR:N    | 3:AC:201:TYR:HD1   | 2.16                     | 0.41              |
| 4:AD:176:LEU:HG   | 4:AD:178:VAL:CG2   | 2.51                     | 0.41              |
| 4:AD:192:GLU:OE2  | 4:AD:192:GLU:HA    | 2.19                     | 0.41              |
| 5:AE:106:PRO:HG2  | 5:AE:107:ARG:H     | 1.86                     | 0.41              |
| 5:AE:84:PHE:O     | 5:AE:86:ALA:N      | 2.53                     | 0.41              |
| 7:AG:80:VAL:HG21  | 7:AG:85:TYR:CE1    | 2.56                     | 0.41              |
| 11:AK:104:GLN:NE2 | 11:AK:106:LYS:HD2  | 2.35                     | 0.41              |
| 11:AK:48:ILE:HG22 | 11:AK:49:GLY:H     | 1.84                     | 0.41              |
| 11:AK:84:VAL:HG12 | 11:AK:95:ILE:HD11  | 2.02                     | 0.41              |
| 13:AM:31:LYS:O    | 13:AM:32:GLU:C     | 2.58                     | 0.41              |
| 13:AM:71:ARG:HB3  | 13:AM:71:ARG:HE    | 1.65                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:91:ARG:HB2   | 13:AM:98:VAL:HG13  | 2.01                     | 0.41              |
| 15:AO:24:SER:OG    | 15:AO:25:THR:N     | 2.54                     | 0.41              |
| 15:AO:76:GLU:C     | 15:AO:78:TYR:N     | 2.72                     | 0.41              |
| 1:AA:376:G:C4'     | 16:AP:5:ARG:HD2    | 2.49                     | 0.41              |
| 17:AQ:29:HIS:O     | 17:AQ:33:GLY:HA2   | 2.20                     | 0.41              |
| 50:B1:57:GLU:C     | 50:B1:58:ILE:CG2   | 2.89                     | 0.41              |
| 50:B1:63:ALA:O     | 50:B1:65:SER:N     | 2.52                     | 0.41              |
| 50:B1:73:LEU:C     | 50:B1:75:GLU:H     | 2.22                     | 0.41              |
| 50:B1:73:LEU:O     | 50:B1:74:VAL:C     | 2.58                     | 0.41              |
| 51:B2:13:ALA:CA    | 51:B2:16:LEU:HD21  | 2.46                     | 0.41              |
| 53:B4:40:ILE:HD13  | 53:B4:48:ILE:O     | 2.20                     | 0.41              |
| 27:BA:1373:A:H2'   | 27:BA:1374:G:H5'   | 2.02                     | 0.41              |
| 27:BA:1464:C:C4    | 27:BA:1465:G:N7    | 2.88                     | 0.41              |
| 27:BA:1545:A:H3'   | 27:BA:1546:C:C6    | 2.54                     | 0.41              |
| 27:BA:1439:A:H61   | 27:BA:1552:G:H1'   | 1.86                     | 0.41              |
| 27:BA:1625:C:C2'   | 27:BA:1626:G:H5'   | 2.50                     | 0.41              |
| 27:BA:1789:A:H2'   | 27:BA:1790:C:O4'   | 2.20                     | 0.41              |
| 27:BA:2074:U:H2'   | 27:BA:2075:U:H6    | 1.82                     | 0.41              |
| 27:BA:2208:A:N3    | 27:BA:2219:G:C2    | 2.89                     | 0.41              |
| 27:BA:2230:G:C4'   | 50:B1:43:TYR:HB2   | 2.50                     | 0.41              |
| 27:BA:2356:C:N4    | 27:BA:2357:U:H3    | 2.18                     | 0.41              |
| 27:BA:2468:G:O2'   | 27:BA:2469:A:P     | 2.78                     | 0.41              |
| 27:BA:2850:A:C6    | 27:BA:2851:A:C5    | 3.09                     | 0.41              |
| 27:BA:29:U:C2      | 27:BA:30:G:C8      | 3.08                     | 0.41              |
| 27:BA:463:G:N2     | 27:BA:466:A:OP2    | 2.51                     | 0.41              |
| 27:BA:813:U:O2'    | 27:BA:1225:G:H1'   | 2.19                     | 0.41              |
| 27:BA:995:C:OP1    | 43:BU:53:ARG:CZ    | 2.68                     | 0.41              |
| 30:BD:246:PRO:CG   | 30:BD:255:LYS:HG3  | 2.40                     | 0.41              |
| 31:BE:172:VAL:HG13 | 31:BE:182:LEU:HD11 | 2.01                     | 0.41              |
| 31:BE:94:GLU:H     | 31:BE:94:GLU:HG2   | 1.59                     | 0.41              |
| 32:BF:164:ARG:CG   | 32:BF:175:THR:OG1  | 2.66                     | 0.41              |
| 33:BG:110:ALA:N    | 33:BG:112:PRO:HD2  | 2.35                     | 0.41              |
| 34:BH:158:HIS:HE1  | 34:BH:168:PRO:C    | 2.24                     | 0.41              |
| 34:BH:19:VAL:HG22  | 34:BH:24:VAL:HG12  | 2.01                     | 0.41              |
| 34:BH:10:PRO:HG3   | 34:BH:50:VAL:H     | 1.84                     | 0.41              |
| 35:BI:112:LYS:N    | 35:BI:114:LEU:HD11 | 2.35                     | 0.41              |
| 35:BI:122:GLU:OE2  | 35:BI:123:LEU:N    | 2.53                     | 0.41              |
| 36:BN:60:ILE:H     | 36:BN:60:ILE:HG13  | 1.52                     | 0.41              |
| 37:BO:7:TYR:HE2    | 37:BO:44:LYS:HG3   | 1.84                     | 0.41              |
| 27:BA:636:G:H2'    | 38:BP:115:LEU:HD12 | 2.02                     | 0.41              |
| 38:BP:132:LYS:O    | 38:BP:136:GLU:HG2  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BP:85:LEU:O    | 38:BP:88:LEU:N    | 2.54                     | 0.41              |
| 39:BQ:133:ARG:O   | 39:BQ:134:ARG:CB  | 2.66                     | 0.41              |
| 40:BR:44:LEU:O    | 40:BR:47:PHE:HB3  | 2.21                     | 0.41              |
| 41:BS:92:TYR:CD1  | 41:BS:93:LYS:N    | 2.82                     | 0.41              |
| 42:BT:78:LEU:HB3  | 42:BT:79:HIS:ND1  | 2.34                     | 0.41              |
| 44:BV:47:VAL:O    | 44:BV:48:GLY:C    | 2.57                     | 0.41              |
| 48:BZ:143:LEU:CD1 | 48:BZ:147:ASP:HB3 | 2.50                     | 0.41              |
| 1:CA:1165:C:H2'   | 1:CA:1166:G:H5'   | 2.01                     | 0.41              |
| 1:CA:1207:G:H2'   | 1:CA:1208:C:C6    | 2.55                     | 0.41              |
| 1:CA:1316:G:N1    | 1:CA:1319:A:OP2   | 2.53                     | 0.41              |
| 1:CA:1346:A:C4    | 1:CA:1348:U:C4    | 3.08                     | 0.41              |
| 1:CA:1375:A:H2'   | 1:CA:1376:U:C6    | 2.55                     | 0.41              |
| 1:CA:178:C:O2'    | 1:CA:179:A:H5'    | 2.20                     | 0.41              |
| 1:CA:276:G:O5'    | 1:CA:276:G:C8     | 2.71                     | 0.41              |
| 1:CA:35:G:N2      | 1:CA:550:G:N3     | 2.69                     | 0.41              |
| 1:CA:404:U:O2'    | 1:CA:405:U:H5'    | 2.19                     | 0.41              |
| 1:CA:460:G:H1     | 1:CA:470:C:H5''   | 1.85                     | 0.41              |
| 1:CA:505:G:H8     | 1:CA:505:G:O5'    | 2.04                     | 0.41              |
| 1:CA:515:G:O2'    | 1:CA:516:U:H5'    | 2.20                     | 0.41              |
| 1:CA:533:A:O2'    | 1:CA:534:U:H3'    | 2.20                     | 0.41              |
| 1:CA:602:A:HO2'   | 1:CA:603:U:H5'    | 1.85                     | 0.41              |
| 1:CA:663:A:O2'    | 1:CA:664:G:H5'    | 2.20                     | 0.41              |
| 1:CA:72:C:C2'     | 1:CA:73:G:H5'     | 2.51                     | 0.41              |
| 1:CA:745:C:H5'    | 1:CA:851:G:H21    | 1.84                     | 0.41              |
| 1:CA:678:U:H1'    | 1:CA:777:A:O3'    | 2.21                     | 0.41              |
| 1:CA:795:C:H5     | 1:CA:796:C:C4     | 2.37                     | 0.41              |
| 1:CA:949:A:C6     | 1:CA:950:U:N3     | 2.89                     | 0.41              |
| 1:CA:970:C:H41    | 9:CI:126:SER:CB   | 2.30                     | 0.41              |
| 2:CB:236:TYR:HA   | 2:CB:239:VAL:CG2  | 2.47                     | 0.41              |
| 4:CD:58:LEU:CD1   | 4:CD:59:ARG:NH1   | 2.84                     | 0.41              |
| 9:CI:106:ALA:O    | 9:CI:108:VAL:HG22 | 2.19                     | 0.41              |
| 10:CJ:61:GLU:HG2  | 14:CN:58:LYS:NZ   | 2.35                     | 0.41              |
| 1:CA:779:C:H4'    | 11:CK:120:ARG:O   | 2.20                     | 0.41              |
| 13:CM:16:ASP:HB2  | 13:CM:31:LYS:CE   | 2.51                     | 0.41              |
| 13:CM:38:GLY:O    | 13:CM:55:ARG:NH2  | 2.54                     | 0.41              |
| 13:CM:81:LEU:HB3  | 13:CM:86:CYS:SG   | 2.61                     | 0.41              |
| 10:CJ:49:VAL:HG21 | 14:CN:41:ARG:HB2  | 2.01                     | 0.41              |
| 1:CA:751:U:C1'    | 15:CO:24:SER:HA   | 2.51                     | 0.41              |
| 17:CQ:21:VAL:HG21 | 17:CQ:59:ILE:HD11 | 2.01                     | 0.41              |
| 17:CQ:55:ASP:OD1  | 17:CQ:79:SER:HA   | 2.20                     | 0.41              |
| 20:CT:51:GLU:H    | 20:CT:51:GLU:HG2  | 1.59                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CX:32:C:C2'     | 24:CX:33:U:H5'     | 2.50                     | 0.41              |
| 25:CY:1:U:O4       | 25:CY:71:A:N1      | 2.53                     | 0.41              |
| 25:CY:26:C:N3      | 25:CY:27:C:N4      | 2.68                     | 0.41              |
| 57:D8:6:THR:CG2    | 57:D8:63:PRO:CG    | 2.97                     | 0.41              |
| 27:DA:1016:G:C6    | 27:DA:1017:G:N7    | 2.89                     | 0.41              |
| 27:DA:1109:C:C5    | 27:DA:1110:G:C4    | 3.08                     | 0.41              |
| 27:DA:1227:G:OP1   | 43:DU:13:LYS:HE2   | 2.20                     | 0.41              |
| 27:DA:1355:G:C6    | 27:DA:1356:G:N7    | 2.89                     | 0.41              |
| 27:DA:1433:U:H1'   | 27:DA:1561:G:N2    | 2.36                     | 0.41              |
| 27:DA:1596:A:C2    | 27:DA:1597:A:C4    | 3.08                     | 0.41              |
| 27:DA:2082:A:H2'   | 27:DA:2083:G:O4'   | 2.19                     | 0.41              |
| 27:DA:2201:C:O2'   | 27:DA:2202:C:H5'   | 2.21                     | 0.41              |
| 27:DA:2293:C:C2    | 27:DA:2340:G:N2    | 2.88                     | 0.41              |
| 27:DA:240:G:O2'    | 27:DA:257:A:N6     | 2.46                     | 0.41              |
| 27:DA:2478:A:N6    | 27:DA:2479:G:C2    | 2.88                     | 0.41              |
| 27:DA:2694:G:C5    | 27:DA:2695:C:C5    | 3.09                     | 0.41              |
| 27:DA:2866:U:C6    | 27:DA:2868:A:H1'   | 2.55                     | 0.41              |
| 27:DA:458:G:O2'    | 27:DA:459:U:P      | 2.79                     | 0.41              |
| 27:DA:464:U:H2'    | 27:DA:465:G:O4'    | 2.20                     | 0.41              |
| 27:DA:524:U:H2'    | 27:DA:525:U:C6     | 2.55                     | 0.41              |
| 27:DA:587:C:N3     | 38:DP:33:ARG:HG2   | 2.35                     | 0.41              |
| 27:DA:632:A:C6     | 27:DA:633:A:N6     | 2.89                     | 0.41              |
| 27:DA:748:G:C6     | 27:DA:750:A:C2     | 3.08                     | 0.41              |
| 27:DA:88:G:OP1     | 27:DA:90:U:C4      | 2.74                     | 0.41              |
| 28:DB:43:C:H3'     | 28:DB:44:G:H5'     | 2.01                     | 0.41              |
| 28:DB:93:G:H2'     | 28:DB:94:C:C6      | 2.54                     | 0.41              |
| 30:DD:186:HIS:HD2  | 30:DD:188:GLU:H    | 1.68                     | 0.41              |
| 30:DD:75:ILE:HA    | 30:DD:76:PRO:HD2   | 1.76                     | 0.41              |
| 31:DE:167:VAL:HG22 | 31:DE:170:LEU:HD11 | 2.03                     | 0.41              |
| 31:DE:175:VAL:O    | 31:DE:177:PRO:HD3  | 2.20                     | 0.41              |
| 32:DF:65:TRP:O     | 32:DF:65:TRP:CE3   | 2.65                     | 0.41              |
| 33:DG:34:LEU:O     | 33:DG:35:GLU:C     | 2.58                     | 0.41              |
| 37:DO:40:VAL:O     | 37:DO:41:ALA:HB2   | 2.20                     | 0.41              |
| 38:DP:111:ARG:NH1  | 38:DP:149:GLU:HG3  | 2.36                     | 0.41              |
| 38:DP:58:THR:C     | 38:DP:61:ARG:NE    | 2.73                     | 0.41              |
| 41:DS:16:ASN:O     | 41:DS:20:ARG:NH2   | 2.53                     | 0.41              |
| 42:DT:120:ARG:O    | 42:DT:123:GLN:HG2  | 2.20                     | 0.41              |
| 42:DT:29:ARG:HD3   | 42:DT:29:ARG:HA    | 1.75                     | 0.41              |
| 42:DT:16:ARG:H     | 42:DT:79:HIS:HD2   | 1.67                     | 0.41              |
| 45:DW:64:MET:O     | 45:DW:65:LEU:CB    | 2.68                     | 0.41              |
| 47:DY:97:ARG:HD2   | 47:DY:97:ARG:HA    | 1.87                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:DZ:22:LYS:HG3  | 48:DZ:38:VAL:O    | 2.20                     | 0.41              |
| 1:AA:1064:G:O2'   | 1:AA:1065:U:P     | 2.79                     | 0.41              |
| 1:AA:1178:G:N7    | 9:AI:97:LYS:HE3   | 2.36                     | 0.41              |
| 1:AA:1258:G:H2'   | 1:AA:1259:C:H6    | 1.85                     | 0.41              |
| 1:AA:169:C:C5     | 1:AA:170:U:H5     | 2.39                     | 0.41              |
| 1:AA:40:C:H2'     | 1:AA:41:G:O4'     | 2.20                     | 0.41              |
| 1:AA:443:C:C2     | 1:AA:444:C:C5     | 3.08                     | 0.41              |
| 1:AA:624:C:O3'    | 16:AP:10:GLY:HA2  | 2.21                     | 0.41              |
| 1:AA:66:G:O4'     | 1:AA:173:U:C4     | 2.73                     | 0.41              |
| 1:AA:69:G:N2      | 1:AA:101:A:C2     | 2.89                     | 0.41              |
| 1:AA:758:G:C2'    | 1:AA:759:A:OP2    | 2.68                     | 0.41              |
| 5:AE:18:ARG:CG    | 5:AE:25:ARG:O     | 2.68                     | 0.41              |
| 6:AF:34:GLY:O     | 6:AF:67:MET:HB2   | 2.20                     | 0.41              |
| 7:AG:118:VAL:O    | 7:AG:121:ALA:HB3  | 2.21                     | 0.41              |
| 1:AA:1118:C:OP1   | 9:AI:104:ARG:NH1  | 2.53                     | 0.41              |
| 10:AJ:43:ARG:HB2  | 10:AJ:67:THR:HG23 | 2.02                     | 0.41              |
| 11:AK:18:ARG:O    | 11:AK:32:ILE:HA   | 2.21                     | 0.41              |
| 14:AN:21:TYR:HD2  | 14:AN:22:THR:O    | 2.03                     | 0.41              |
| 15:AO:23:GLY:C    | 15:AO:24:SER:O    | 2.58                     | 0.41              |
| 20:AT:74:LYS:C    | 20:AT:76:ALA:H    | 2.22                     | 0.41              |
| 20:AT:87:LYS:O    | 20:AT:91:LEU:CG   | 2.66                     | 0.41              |
| 20:AT:56:MET:SD   | 20:AT:88:VAL:HG21 | 2.60                     | 0.41              |
| 50:B1:45:ASN:HD22 | 50:B1:45:ASN:HA   | 1.64                     | 0.41              |
| 50:B1:83:GLU:O    | 50:B1:84:GLY:O    | 2.39                     | 0.41              |
| 51:B2:24:LEU:CD1  | 51:B2:28:LYS:HE2  | 2.50                     | 0.41              |
| 52:B3:29:ARG:HB2  | 52:B3:30:ARG:CD   | 2.50                     | 0.41              |
| 52:B3:54:VAL:HG12 | 52:B3:56:VAL:HG22 | 2.03                     | 0.41              |
| 38:BP:65:ARG:HH21 | 57:B8:15:LYS:HD2  | 1.84                     | 0.41              |
| 57:B8:28:GLY:O    | 57:B8:32:LEU:CD2  | 2.61                     | 0.41              |
| 27:BA:1218:C:H42  | 27:BA:1231:G:H1   | 1.68                     | 0.41              |
| 27:BA:1797:C:C5'  | 30:BD:257:LEU:O   | 2.68                     | 0.41              |
| 27:BA:1866:C:H6   | 27:BA:1866:C:O5'  | 2.04                     | 0.41              |
| 27:BA:2025:C:H2'  | 27:BA:2026:C:C6   | 2.55                     | 0.41              |
| 27:BA:2079:U:O3'  | 50:B1:35:THR:OG1  | 2.26                     | 0.41              |
| 27:BA:2261:C:C2   | 27:BA:2280:G:N2   | 2.89                     | 0.41              |
| 27:BA:2649:U:O2'  | 27:BA:2650:U:H5'  | 2.19                     | 0.41              |
| 27:BA:489:G:C2    | 27:BA:491:G:C4    | 3.09                     | 0.41              |
| 27:BA:27:G:H1'    | 27:BA:513:A:N6    | 2.34                     | 0.41              |
| 27:BA:538:G:C6    | 27:BA:539:G:N7    | 2.88                     | 0.41              |
| 27:BA:847:U:O4    | 27:BA:933:A:N6    | 2.54                     | 0.41              |
| 28:BB:42:C:C5     | 28:BB:43:C:C5     | 3.08                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:BC:19:VAL:CG1  | 29:BC:20:TYR:HD1  | 2.30                     | 0.41              |
| 29:BC:36:LYS:HZ3  | 29:BC:36:LYS:HB2  | 1.86                     | 0.41              |
| 30:BD:226:MET:SD  | 30:BD:230:ASP:HB3 | 2.59                     | 0.41              |
| 31:BE:3:GLY:HA3   | 31:BE:81:ILE:HG21 | 2.01                     | 0.41              |
| 34:BH:142:GLY:O   | 34:BH:143:GLN:C   | 2.57                     | 0.41              |
| 36:BN:36:GLY:H    | 36:BN:48:MET:HE3  | 1.85                     | 0.41              |
| 37:BO:77:ILE:HG13 | 37:BO:78:ARG:N    | 2.36                     | 0.41              |
| 39:BQ:65:PHE:HB2  | 39:BQ:105:GLU:CG  | 2.46                     | 0.41              |
| 40:BR:10:LEU:CA   | 40:BR:17:ARG:HD2  | 2.44                     | 0.41              |
| 37:BO:77:ILE:CD1  | 42:BT:74:ARG:HG2  | 2.51                     | 0.41              |
| 43:BU:111:GLU:O   | 43:BU:112:ARG:C   | 2.58                     | 0.41              |
| 44:BV:47:VAL:O    | 44:BV:49:THR:N    | 2.53                     | 0.41              |
| 44:BV:64:HIS:ND1  | 44:BV:92:THR:HB   | 2.36                     | 0.41              |
| 45:BW:52:GLU:O    | 45:BW:55:ALA:HB3  | 2.20                     | 0.41              |
| 1:CA:1058:G:O2'   | 1:CA:1059:C:H5'   | 2.21                     | 0.41              |
| 1:CA:1132:C:HO2'  | 1:CA:1133:G:H5'   | 1.81                     | 0.41              |
| 1:CA:129(A):G:C2  | 1:CA:189(H):G:C8  | 3.08                     | 0.41              |
| 1:CA:1316:G:N2    | 1:CA:1319:A:OP2   | 2.53                     | 0.41              |
| 1:CA:1518:A:H2'   | 1:CA:1519:A:O4'   | 2.20                     | 0.41              |
| 1:CA:590:C:OP1    | 8:CH:30:ARG:N     | 2.49                     | 0.41              |
| 1:CA:643:C:H5'    | 8:CH:31:PHE:CG    | 2.55                     | 0.41              |
| 1:CA:860:A:H4'    | 8:CH:75:ARG:HH22  | 1.86                     | 0.41              |
| 1:CA:9:G:OP1      | 5:CE:122:GLU:CB   | 2.68                     | 0.41              |
| 1:CA:1191:A:C5'   | 3:CC:4:LYS:HZ1    | 2.32                     | 0.41              |
| 4:CD:8:VAL:HG11   | 4:CD:21:LEU:CB    | 2.51                     | 0.41              |
| 5:CE:143:ARG:O    | 5:CE:144:THR:O    | 2.38                     | 0.41              |
| 5:CE:78:HIS:HB2   | 5:CE:79:GLU:H     | 1.69                     | 0.41              |
| 6:CF:10:LEU:HD21  | 6:CF:26:ILE:HD11  | 2.02                     | 0.41              |
| 1:CA:736:C:H4'    | 6:CF:91:VAL:HG22  | 2.01                     | 0.41              |
| 12:CL:53:ALA:O    | 12:CL:65:ALA:N    | 2.34                     | 0.41              |
| 13:CM:58:GLU:O    | 13:CM:59:TYR:C    | 2.59                     | 0.41              |
| 14:CN:45:ARG:O    | 14:CN:46:GLU:C    | 2.59                     | 0.41              |
| 19:CS:22:LEU:HD13 | 19:CS:27:GLU:HB2  | 2.01                     | 0.41              |
| 20:CT:25:ARG:CZ   | 20:CT:25:ARG:HB2  | 2.51                     | 0.41              |
| 24:CX:37:A:H2'    | 24:CX:38:A:O4'    | 2.20                     | 0.41              |
| 27:DA:381:G:OP1   | 50:D1:16:ASN:HB2  | 2.20                     | 0.41              |
| 52:D3:47:VAL:CA   | 52:D3:50:VAL:HG22 | 2.51                     | 0.41              |
| 52:D3:6:VAL:O     | 52:D3:34:GLU:HB3  | 2.20                     | 0.41              |
| 56:D7:30:VAL:O    | 56:D7:31:LEU:C    | 2.58                     | 0.41              |
| 27:DA:1111:A:O2'  | 27:DA:1112:G:H4'  | 2.21                     | 0.41              |
| 27:DA:1424:G:C6   | 27:DA:1425:G:C4   | 3.08                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:1482:G:H2'  | 27:DA:1484:G:O4'   | 2.20                     | 0.41              |
| 27:DA:1578:U:C2'  | 27:DA:1579:A:H5''  | 2.49                     | 0.41              |
| 27:DA:1838:C:H6   | 27:DA:1838:C:H2'   | 1.64                     | 0.41              |
| 27:DA:1999:C:H2'  | 27:DA:2000:G:H8    | 1.85                     | 0.41              |
| 27:DA:2255:G:C6   | 27:DA:2256:G:C5    | 3.08                     | 0.41              |
| 27:DA:2301:C:C3'  | 27:DA:2301:C:C6    | 3.04                     | 0.41              |
| 27:DA:2509:G:N2   | 27:DA:2580:U:C2    | 2.89                     | 0.41              |
| 27:DA:2591:C:OP1  | 30:DD:239:ARG:NH2  | 2.54                     | 0.41              |
| 27:DA:2748:A:O2'  | 34:DH:63:SER:HA    | 2.20                     | 0.41              |
| 27:DA:2811:G:OP2  | 27:DA:2811:G:H8    | 2.04                     | 0.41              |
| 27:DA:494:G:H2'   | 27:DA:495:G:C8     | 2.56                     | 0.41              |
| 27:DA:555:U:C2'   | 27:DA:556:G:H8     | 2.33                     | 0.41              |
| 27:DA:662:G:H5''  | 38:DP:18:ARG:C     | 2.39                     | 0.41              |
| 27:DA:870:A:C2    | 27:DA:871:U:C2     | 3.08                     | 0.41              |
| 28:DB:31:C:C5'    | 28:DB:32:C:OP2     | 2.69                     | 0.41              |
| 29:DC:20:TYR:N    | 29:DC:20:TYR:CD1   | 2.88                     | 0.41              |
| 29:DC:59:ARG:HB2  | 29:DC:62:VAL:HG22  | 2.03                     | 0.41              |
| 31:DE:175:VAL:O   | 31:DE:175:VAL:CG2  | 2.68                     | 0.41              |
| 32:DF:3:GLU:HB3   | 32:DF:24:LEU:HG    | 2.03                     | 0.41              |
| 34:DH:152:ARG:HB2 | 34:DH:162:ILE:HD11 | 2.03                     | 0.41              |
| 36:DN:104:LYS:C   | 36:DN:106:MET:H    | 2.23                     | 0.41              |
| 38:DP:49:ARG:HD2  | 57:D8:58:ILE:HG22  | 2.00                     | 0.41              |
| 28:DB:91:C:OP1    | 39:DQ:16:ARG:HG3   | 2.20                     | 0.41              |
| 41:DS:102:ALA:O   | 41:DS:104:GLY:N    | 2.54                     | 0.41              |
| 42:DT:74:ARG:HD3  | 42:DT:76:PHE:HE2   | 1.82                     | 0.41              |
| 42:DT:83:ILE:CG1  | 42:DT:84:GLN:N     | 2.80                     | 0.41              |
| 43:DU:35:ALA:O    | 43:DU:38:THR:HB    | 2.20                     | 0.41              |
| 36:DN:2:LYS:CE    | 44:DV:13:ARG:HB3   | 2.49                     | 0.41              |
| 43:DU:90:VAL:HG21 | 44:DV:47:VAL:HG21  | 2.03                     | 0.41              |
| 45:DW:51:LEU:O    | 45:DW:54:ALA:HB3   | 2.20                     | 0.41              |
| 46:DX:35:THR:CG2  | 46:DX:37:THR:HB    | 2.50                     | 0.41              |
| 47:DY:26:LYS:HZ2  | 47:DY:27:VAL:HG23  | 1.86                     | 0.41              |
| 27:DA:480:A:P     | 47:DY:46:LYS:HE2   | 2.60                     | 0.41              |
| 47:DY:54:LYS:C    | 47:DY:55:TYR:CG    | 2.94                     | 0.41              |
| 1:AA:1258:G:C5    | 1:AA:1259:C:H5     | 2.38                     | 0.41              |
| 1:AA:1271:G:H2'   | 1:AA:1272:G:C8     | 2.54                     | 0.41              |
| 1:AA:1321:C:H5'   | 1:AA:1322:C:H5'    | 1.99                     | 0.41              |
| 1:AA:136:C:H42    | 1:AA:227:G:H1      | 1.68                     | 0.41              |
| 1:AA:244:U:O4     | 1:AA:893:C:N3      | 2.52                     | 0.41              |
| 1:AA:299:G:C5     | 1:AA:300:A:C6      | 3.08                     | 0.41              |
| 1:AA:344:A:C2'    | 1:AA:346:G:O6      | 2.67                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:355:C:C2'    | 1:AA:356:A:O5'    | 2.69                     | 0.41              |
| 1:AA:461:A:C5     | 1:AA:471:G:C5     | 3.09                     | 0.41              |
| 1:AA:577:G:O2'    | 1:AA:578:C:C5'    | 2.68                     | 0.41              |
| 1:AA:619:U:C4     | 4:AD:135:LEU:HD11 | 2.55                     | 0.41              |
| 1:AA:652:U:O2'    | 1:AA:653:A:C5'    | 2.69                     | 0.41              |
| 1:AA:683:G:H21    | 11:AK:38:ASN:HA   | 1.86                     | 0.41              |
| 1:AA:704:A:C2     | 1:AA:705:U:C2     | 3.08                     | 0.41              |
| 2:AB:8:LYS:N      | 2:AB:8:LYS:HD3    | 2.36                     | 0.41              |
| 3:AC:64:VAL:CG2   | 3:AC:99:VAL:HA    | 2.51                     | 0.41              |
| 4:AD:16:GLY:O     | 4:AD:17:VAL:C     | 2.59                     | 0.41              |
| 4:AD:28:SER:C     | 4:AD:30:LYS:H     | 2.23                     | 0.41              |
| 6:AF:89:MET:SD    | 18:AR:76:LEU:CD2  | 3.06                     | 0.41              |
| 6:AF:9:VAL:CG2    | 6:AF:60:PHE:CE2   | 3.04                     | 0.41              |
| 8:AH:14:ARG:O     | 8:AH:16:ALA:N     | 2.54                     | 0.41              |
| 10:AJ:78:ASN:ND2  | 10:AJ:81:THR:H    | 2.18                     | 0.41              |
| 11:AK:123:LYS:O   | 11:AK:126:ARG:HB2 | 2.21                     | 0.41              |
| 13:AM:70:LEU:O    | 13:AM:73:GLU:HB3  | 2.20                     | 0.41              |
| 18:AR:37:VAL:O    | 18:AR:39:VAL:N    | 2.54                     | 0.41              |
| 19:AS:6:LYS:HD2   | 19:AS:7:LYS:HE3   | 2.02                     | 0.41              |
| 22:AV:7:C:N3      | 23:AW:36:A:C2     | 2.88                     | 0.41              |
| 1:AA:1492:A:H3'   | 26:AZ:6:5OH:HNP   | 1.86                     | 0.41              |
| 49:B0:31:VAL:HG22 | 49:B0:65:GLY:O    | 2.20                     | 0.41              |
| 55:B6:19:ARG:CG   | 55:B6:20:ASN:N    | 2.76                     | 0.41              |
| 27:BA:1111:A:C2'  | 27:BA:1112:G:H4'  | 2.49                     | 0.41              |
| 27:BA:1175:U:C2'  | 27:BA:1175:U:O2   | 2.67                     | 0.41              |
| 27:BA:1278:A:HO2' | 27:BA:1279:G:H5'  | 1.85                     | 0.41              |
| 27:BA:1464:C:O2'  | 27:BA:1465:G:H5'  | 2.21                     | 0.41              |
| 27:BA:1518:U:O4   | 27:BA:1519:G:C6   | 2.73                     | 0.41              |
| 27:BA:1816:G:H2'  | 30:BD:62:TYR:CE2  | 2.55                     | 0.41              |
| 27:BA:1877:A:H5'' | 27:BA:1878:G:OP2  | 2.21                     | 0.41              |
| 27:BA:2224:G:O2'  | 27:BA:2225:A:O4'  | 2.39                     | 0.41              |
| 27:BA:2416:C:H2'  | 27:BA:2417:C:C6   | 2.55                     | 0.41              |
| 27:BA:2476:A:N1   | 27:BA:2477:C:C6   | 2.88                     | 0.41              |
| 27:BA:257:A:H2'   | 27:BA:258:G:C5'   | 2.50                     | 0.41              |
| 27:BA:2653:U:OP2  | 27:BA:2654:A:H3'  | 2.20                     | 0.41              |
| 27:BA:2752:C:H5'  | 27:BA:2753:A:OP2  | 2.21                     | 0.41              |
| 27:BA:382:G:H2'   | 27:BA:383:U:C5'   | 2.48                     | 0.41              |
| 27:BA:385:C:O2'   | 27:BA:388:G:N2    | 2.54                     | 0.41              |
| 27:BA:508:G:C5'   | 27:BA:509:C:OP1   | 2.69                     | 0.41              |
| 27:BA:829:A:N7    | 27:BA:2248:C:H5'  | 2.35                     | 0.41              |
| 27:BA:952:G:C6    | 27:BA:966:G:C6    | 3.08                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:978:G:O4'    | 27:BA:1001:A:H2    | 2.03                     | 0.41              |
| 29:BC:182:PRO:O    | 29:BC:183:GLU:CB   | 2.69                     | 0.41              |
| 30:BD:12:SER:OG    | 30:BD:13:ARG:N     | 2.53                     | 0.41              |
| 30:BD:202:LYS:HG3  | 30:BD:203:ASN:OD1  | 2.20                     | 0.41              |
| 30:BD:257:LEU:HA   | 30:BD:257:LEU:HD23 | 1.82                     | 0.41              |
| 31:BE:38:THR:HB    | 31:BE:40:GLU:CD    | 2.41                     | 0.41              |
| 31:BE:64:LYS:HG2   | 31:BE:64:LYS:O     | 2.20                     | 0.41              |
| 32:BF:202:PHE:HA   | 32:BF:205:ARG:HB3  | 2.01                     | 0.41              |
| 24:AX:56:C:H1'     | 33:BG:76:SER:CB    | 2.51                     | 0.41              |
| 34:BH:115:VAL:HG21 | 34:BH:148:ILE:CD1  | 2.50                     | 0.41              |
| 35:BI:101:LEU:HD23 | 35:BI:109:ILE:HD11 | 2.03                     | 0.41              |
| 35:BI:22:LYS:O     | 35:BI:23:PRO:C     | 2.59                     | 0.41              |
| 36:BN:94:HIS:O     | 36:BN:95:PRO:C     | 2.57                     | 0.41              |
| 37:BO:36:GLY:CA    | 37:BO:109:LYS:HG3  | 2.50                     | 0.41              |
| 37:BO:19:ILE:CG2   | 37:BO:43:VAL:HG13  | 2.41                     | 0.41              |
| 38:BP:30:THR:CG2   | 38:BP:31:ALA:H     | 2.14                     | 0.41              |
| 38:BP:41:ARG:HE    | 38:BP:45:LEU:HD12  | 1.86                     | 0.41              |
| 39:BQ:56:ARG:O     | 39:BQ:57:HIS:C     | 2.56                     | 0.41              |
| 41:BS:15:ARG:O     | 41:BS:17:ARG:O     | 2.38                     | 0.41              |
| 41:BS:87:PHE:CD2   | 41:BS:88:ASP:N     | 2.65                     | 0.41              |
| 42:BT:106:SER:HB3  | 42:BT:110:ILE:HD12 | 1.98                     | 0.41              |
| 42:BT:35:LYS:HG3   | 42:BT:36:GLU:HB2   | 2.03                     | 0.41              |
| 44:BV:91:TYR:C     | 44:BV:91:TYR:CD1   | 2.94                     | 0.41              |
| 45:BW:47:VAL:O     | 45:BW:50:VAL:CG1   | 2.69                     | 0.41              |
| 46:BX:50:LYS:HE3   | 46:BX:84:ALA:HB2   | 2.02                     | 0.41              |
| 47:BY:28:LYS:CB    | 47:BY:38:ILE:H     | 2.33                     | 0.41              |
| 47:BY:46:LYS:CG    | 47:BY:47:LYS:HE3   | 2.49                     | 0.41              |
| 48:BZ:117:GLN:HG2  | 48:BZ:119:ILE:HG13 | 2.02                     | 0.41              |
| 1:CA:1194:U:N3     | 1:CA:1195:C:C4     | 2.89                     | 0.41              |
| 1:CA:1275:A:H2'    | 1:CA:1276:G:O4'    | 2.20                     | 0.41              |
| 1:CA:1281:U:H5'    | 1:CA:1282:C:OP2    | 2.21                     | 0.41              |
| 1:CA:1255:G:C5     | 1:CA:1283:G:N2     | 2.89                     | 0.41              |
| 1:CA:1483:A:H3'    | 1:CA:1484:C:H6     | 1.86                     | 0.41              |
| 1:CA:1509:C:O2'    | 1:CA:1510:U:H5'    | 2.21                     | 0.41              |
| 1:CA:189(D):C:H2'  | 1:CA:189(E):U:C1'  | 2.51                     | 0.41              |
| 1:CA:31:G:N2       | 1:CA:47:C:O5'      | 2.53                     | 0.41              |
| 1:CA:47:C:O2'      | 1:CA:48:C:P        | 2.78                     | 0.41              |
| 1:CA:678:U:N3      | 1:CA:713:G:N2      | 2.69                     | 0.41              |
| 1:CA:758:G:H8      | 1:CA:758:G:O5'     | 2.03                     | 0.41              |
| 1:CA:961:U:C4      | 1:CA:983:A:C6      | 3.09                     | 0.41              |
| 2:CB:85:ALA:CB     | 2:CB:92:TYR:HD2    | 2.33                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CC:177:THR:HG22 | 3:CC:179:ARG:HG2  | 2.01                     | 0.41              |
| 4:CD:19:LEU:O     | 4:CD:26:CYS:SG    | 2.78                     | 0.41              |
| 5:CE:110:LEU:HD21 | 5:CE:139:LEU:HD11 | 2.02                     | 0.41              |
| 5:CE:7:GLU:HB2    | 5:CE:35:GLY:O     | 2.21                     | 0.41              |
| 6:CF:25:ILE:HD13  | 6:CF:25:ILE:HA    | 1.91                     | 0.41              |
| 7:CG:115:ARG:O    | 7:CG:116:ALA:C    | 2.58                     | 0.41              |
| 7:CG:146:GLU:CA   | 7:CG:149:ARG:HB2  | 2.51                     | 0.41              |
| 8:CH:109:ILE:HG23 | 8:CH:110:ALA:N    | 2.35                     | 0.41              |
| 8:CH:38:ILE:C     | 8:CH:40:ALA:N     | 2.74                     | 0.41              |
| 10:CJ:35:SER:O    | 10:CJ:36:GLY:C    | 2.59                     | 0.41              |
| 12:CL:59:SER:C    | 12:CL:61:TYR:H    | 2.23                     | 0.41              |
| 12:CL:61:TYR:O    | 12:CL:62:GLU:HB2  | 2.20                     | 0.41              |
| 15:CO:61:GLY:O    | 15:CO:65:ARG:CD   | 2.67                     | 0.41              |
| 15:CO:71:GLN:HE21 | 15:CO:71:GLN:HB3  | 1.70                     | 0.41              |
| 15:CO:83:GLU:C    | 15:CO:85:LEU:N    | 2.73                     | 0.41              |
| 17:CQ:78:GLU:CD   | 17:CQ:81:ARG:HD2  | 2.39                     | 0.41              |
| 20:CT:86:ARG:NH1  | 20:CT:86:ARG:HG3  | 2.31                     | 0.41              |
| 21:CU:9:ARG:C     | 21:CU:11:GLY:H    | 2.23                     | 0.41              |
| 27:DA:747:U:C4    | 54:D5:2:ALA:N     | 2.88                     | 0.41              |
| 27:DA:2344:U:OP1  | 55:D6:38:LYS:HD2  | 2.20                     | 0.41              |
| 57:D8:62:LEU:N    | 57:D8:63:PRO:CD   | 2.82                     | 0.41              |
| 27:DA:1267:U:O2'  | 27:DA:1268:A:O5'  | 2.38                     | 0.41              |
| 27:DA:1334:G:O2'  | 27:DA:1335:U:H5'  | 2.20                     | 0.41              |
| 27:DA:1348:G:C5   | 27:DA:1349:A:C2   | 3.08                     | 0.41              |
| 27:DA:1408:C:C2   | 27:DA:1595:G:N2   | 2.88                     | 0.41              |
| 27:DA:1495:A:H8   | 27:DA:1495:A:OP1  | 2.03                     | 0.41              |
| 27:DA:1562:A:C2   | 27:DA:1563:G:C4   | 3.09                     | 0.41              |
| 27:DA:1578:U:O2   | 27:DA:1578:U:C2'  | 2.69                     | 0.41              |
| 27:DA:1586:A:C2   | 27:DA:1587:A:C5   | 3.09                     | 0.41              |
| 27:DA:1591:G:O2'  | 27:DA:1592:C:H5'  | 2.21                     | 0.41              |
| 27:DA:1684:C:N3   | 27:DA:1704:G:O6   | 2.54                     | 0.41              |
| 27:DA:175:G:O2'   | 27:DA:176:G:H5'   | 2.21                     | 0.41              |
| 27:DA:1862:G:C2   | 27:DA:1863:G:C5   | 3.09                     | 0.41              |
| 27:DA:1941:C:C4   | 27:DA:1965:C:C6   | 3.09                     | 0.41              |
| 27:DA:2050:C:H1'  | 31:DE:156:MET:CE  | 2.51                     | 0.41              |
| 27:DA:2102:U:H5'  | 27:DA:2103:C:P    | 2.61                     | 0.41              |
| 27:DA:2156:G:C6   | 27:DA:2157:G:N2   | 2.89                     | 0.41              |
| 27:DA:216:A:C2    | 27:DA:217:G:C4    | 3.09                     | 0.41              |
| 27:DA:21:A:C2     | 27:DA:22:C:O2     | 2.74                     | 0.41              |
| 27:DA:2526:G:N3   | 58:D9:2:LYS:HE2   | 2.35                     | 0.41              |
| 27:DA:2507:C:C4   | 27:DA:2583:G:N1   | 2.89                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2790:A:C2    | 27:DA:2791:C:H3'   | 2.55                     | 0.41              |
| 27:DA:2832:U:C4'   | 27:DA:2833:G:H5''  | 2.45                     | 0.41              |
| 27:DA:2840:C:O2'   | 40:DR:91:GLN:HG2   | 2.20                     | 0.41              |
| 27:DA:499:U:H3'    | 27:DA:499:U:H6     | 1.86                     | 0.41              |
| 27:DA:52:A:C2      | 27:DA:53:A:C5      | 3.09                     | 0.41              |
| 27:DA:661:C:H2'    | 27:DA:662:G:C8     | 2.54                     | 0.41              |
| 27:DA:745:G:OP1    | 31:DE:133:LYS:NZ   | 2.44                     | 0.41              |
| 27:DA:74:A:H2'     | 27:DA:74:A:N3      | 2.36                     | 0.41              |
| 27:DA:771:G:H2'    | 27:DA:772:C:H6     | 1.86                     | 0.41              |
| 27:DA:797:C:OP1    | 32:DF:60:SER:OG    | 2.31                     | 0.41              |
| 27:DA:873:G:O2'    | 27:DA:874:G:H5'    | 2.20                     | 0.41              |
| 27:DA:963:U:H2'    | 27:DA:964:C:C6     | 2.55                     | 0.41              |
| 27:DA:995:C:O2'    | 27:DA:996:A:OP2    | 2.38                     | 0.41              |
| 29:DC:61:THR:HA    | 29:DC:164:ARG:HA   | 2.01                     | 0.41              |
| 30:DD:208:LYS:HG2  | 30:DD:210:GLY:C    | 2.40                     | 0.41              |
| 27:DA:1971:A:C2    | 30:DD:239:ARG:O    | 2.73                     | 0.41              |
| 27:DA:1797:C:H4'   | 30:DD:257:LEU:O    | 2.20                     | 0.41              |
| 27:DA:773:U:C4'    | 30:DD:47:GLY:HA3   | 2.50                     | 0.41              |
| 31:DE:150:VAL:O    | 31:DE:151:TYR:C    | 2.58                     | 0.41              |
| 32:DF:164:ARG:HG2  | 32:DF:164:ARG:NH1  | 2.36                     | 0.41              |
| 33:DG:111:LEU:HD23 | 33:DG:114:ILE:HD11 | 2.03                     | 0.41              |
| 35:DI:43:ASN:O     | 35:DI:46:ALA:HB3   | 2.21                     | 0.41              |
| 37:DO:35:VAL:HA    | 37:DO:62:VAL:CG1   | 2.50                     | 0.41              |
| 39:DQ:108:GLY:O    | 39:DQ:109:VAL:HB   | 2.21                     | 0.41              |
| 27:DA:958:U:H3     | 39:DQ:17:LEU:HD11  | 1.85                     | 0.41              |
| 40:DR:41:ALA:O     | 40:DR:43:GLU:N     | 2.53                     | 0.41              |
| 40:DR:74:LYS:O     | 40:DR:76:VAL:N     | 2.53                     | 0.41              |
| 42:DT:32:TYR:O     | 42:DT:33:LYS:HB2   | 2.21                     | 0.41              |
| 42:DT:54:ARG:O     | 42:DT:55:ASN:HB2   | 2.20                     | 0.41              |
| 43:DU:103:PRO:O    | 43:DU:104:GLN:C    | 2.57                     | 0.41              |
| 43:DU:21:ALA:HA    | 43:DU:24:TYR:CE1   | 2.55                     | 0.41              |
| 43:DU:35:ALA:O     | 43:DU:39:LEU:HG    | 2.21                     | 0.41              |
| 44:DV:81:TYR:HE2   | 44:DV:83:ARG:CZ    | 2.32                     | 0.41              |
| 48:DZ:115:VAL:O    | 48:DZ:116:LEU:C    | 2.59                     | 0.41              |
| 1:AA:1053:G:O2'    | 1:AA:1199:U:H5     | 2.03                     | 0.41              |
| 1:AA:1055:A:C6     | 1:AA:1206:G:C5     | 3.08                     | 0.41              |
| 1:AA:1404:C:O2'    | 1:AA:1405:G:H5'    | 2.21                     | 0.41              |
| 1:AA:1422:G:H2'    | 1:AA:1423:G:C8     | 2.55                     | 0.41              |
| 1:AA:255:G:N2      | 1:AA:272:C:C2      | 2.88                     | 0.41              |
| 1:AA:301:G:H5''    | 1:AA:301:G:H8      | 1.86                     | 0.41              |
| 1:AA:322:C:O2'     | 1:AA:323:U:H5'     | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:70:G:C6      | 1:AA:71:C:C4      | 3.09                     | 0.41              |
| 1:AA:767:A:O5'    | 1:AA:767:A:H8     | 2.04                     | 0.41              |
| 1:AA:759:A:H4'    | 1:AA:881:G:OP1    | 2.21                     | 0.41              |
| 1:AA:955:U:O2'    | 1:AA:956:U:H5'    | 2.21                     | 0.41              |
| 2:AB:132:LYS:HA   | 2:AB:135:GLN:CG   | 2.50                     | 0.41              |
| 3:AC:28:GLN:HB3   | 3:AC:28:GLN:HE21  | 1.56                     | 0.41              |
| 4:AD:201:GLN:OE1  | 4:AD:204:ILE:HG13 | 2.21                     | 0.41              |
| 4:AD:4:TYR:HE2    | 4:AD:7:PRO:O      | 2.03                     | 0.41              |
| 6:AF:21:LEU:HA    | 6:AF:21:LEU:HD13  | 1.90                     | 0.41              |
| 7:AG:23:VAL:CG1   | 7:AG:27:ILE:HD11  | 2.48                     | 0.41              |
| 9:AI:53:VAL:HG12  | 9:AI:92:TYR:CD2   | 2.55                     | 0.41              |
| 10:AJ:5:ARG:HG3   | 10:AJ:71:LEU:HD11 | 2.03                     | 0.41              |
| 10:AJ:78:ASN:HD22 | 10:AJ:80:LYS:CB   | 2.34                     | 0.41              |
| 11:AK:52:GLY:H    | 11:AK:55:LYS:HG3  | 1.86                     | 0.41              |
| 1:AA:522:C:H5''   | 12:AL:117:TYR:OH  | 2.21                     | 0.41              |
| 12:AL:21:VAL:HG11 | 12:AL:23:ALA:HB2  | 2.00                     | 0.41              |
| 12:AL:38:ARG:NH2  | 12:AL:54:LYS:HZ3  | 2.17                     | 0.41              |
| 14:AN:45:ARG:O    | 14:AN:49:HIS:HD2  | 2.03                     | 0.41              |
| 1:AA:128:G:H5''   | 17:AQ:2:PRO:HA    | 2.03                     | 0.41              |
| 20:AT:29:LYS:HA   | 20:AT:32:ALA:HB3  | 2.03                     | 0.41              |
| 20:AT:57:ARG:O    | 20:AT:58:LYS:C    | 2.59                     | 0.41              |
| 20:AT:63:ILE:C    | 20:AT:65:LYS:N    | 2.74                     | 0.41              |
| 50:B1:58:ILE:HD11 | 50:B1:60:PHE:CZ   | 2.55                     | 0.41              |
| 56:B7:29:LYS:NZ   | 56:B7:32:LYS:NZ   | 2.68                     | 0.41              |
| 58:B9:8:LYS:O     | 58:B9:34:GLN:OE1  | 2.38                     | 0.41              |
| 27:BA:1048:A:O2'  | 27:BA:1049:C:O5'  | 2.36                     | 0.41              |
| 27:BA:1315:C:H2'  | 27:BA:1316:U:H5'  | 2.01                     | 0.41              |
| 27:BA:1773:A:H2'  | 27:BA:1774:C:H5'  | 2.03                     | 0.41              |
| 27:BA:1796:U:H2'  | 27:BA:1797:C:C6   | 2.55                     | 0.41              |
| 27:BA:1891:G:C4   | 27:BA:1892:C:C5   | 3.08                     | 0.41              |
| 26:AZ:4:SER:O     | 27:BA:1914:C:OP2  | 2.39                     | 0.41              |
| 27:BA:2019:A:C2'  | 27:BA:2020:A:O5'  | 2.69                     | 0.41              |
| 27:BA:2228:G:H2'  | 27:BA:2229:C:C6   | 2.56                     | 0.41              |
| 27:BA:2248:C:H2'  | 27:BA:2249:U:O4'  | 2.21                     | 0.41              |
| 27:BA:2276:G:O2'  | 27:BA:2277:G:H5'  | 2.21                     | 0.41              |
| 27:BA:2287:A:C4   | 27:BA:2289:G:C8   | 3.08                     | 0.41              |
| 27:BA:2358:G:C5   | 27:BA:2359:C:C5   | 3.09                     | 0.41              |
| 27:BA:2437:U:H2'  | 27:BA:2438:U:C6   | 2.56                     | 0.41              |
| 27:BA:2468:G:OP1  | 39:BQ:119:ARG:NH1 | 2.45                     | 0.41              |
| 27:BA:2725:A:O2'  | 27:BA:2726:U:C2   | 2.73                     | 0.41              |
| 27:BA:2842:G:C6   | 27:BA:2876:G:C6   | 3.09                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:286:C:C3'    | 27:BA:287:C:H5'    | 2.48                     | 0.41              |
| 27:BA:382:G:H1     | 27:BA:392:C:N4     | 2.18                     | 0.41              |
| 27:BA:383:U:H5     | 27:BA:385:C:H3'    | 1.86                     | 0.41              |
| 27:BA:754:C:H6     | 27:BA:754:C:C5'    | 2.33                     | 0.41              |
| 29:BC:78:ALA:CB    | 29:BC:82:LYS:HB2   | 2.51                     | 0.41              |
| 29:BC:82:LYS:O     | 29:BC:86:ALA:HB3   | 2.20                     | 0.41              |
| 30:BD:65:ILE:HG13  | 30:BD:105:ILE:HA   | 2.02                     | 0.41              |
| 30:BD:143:HIS:N    | 30:BD:143:HIS:ND1  | 2.68                     | 0.41              |
| 30:BD:212:SER:O    | 30:BD:217:ARG:HB2  | 2.21                     | 0.41              |
| 30:BD:54:ARG:O     | 30:BD:218:ARG:HG3  | 2.21                     | 0.41              |
| 27:BA:781:A:OP1    | 30:BD:218:ARG:NH2  | 2.54                     | 0.41              |
| 30:BD:261:LYS:CE   | 30:BD:263:ARG:HH22 | 2.32                     | 0.41              |
| 27:BA:1800:C:P     | 30:BD:266:SER:HG   | 2.44                     | 0.41              |
| 31:BE:105:THR:HG21 | 31:BE:164:ARG:HH12 | 1.82                     | 0.41              |
| 31:BE:176:ILE:N    | 31:BE:176:ILE:HD12 | 2.36                     | 0.41              |
| 31:BE:9:VAL:CG1    | 31:BE:25:VAL:O     | 2.65                     | 0.41              |
| 31:BE:1:MET:CB     | 31:BE:83:ASP:O     | 2.68                     | 0.41              |
| 31:BE:93:VAL:C     | 31:BE:95:ILE:N     | 2.68                     | 0.41              |
| 32:BF:33:LEU:HD13  | 32:BF:112:MET:CE   | 2.49                     | 0.41              |
| 33:BG:125:PHE:CG   | 33:BG:131:TYR:HD1  | 2.38                     | 0.41              |
| 34:BH:157:TYR:O    | 34:BH:158:HIS:HB2  | 2.20                     | 0.41              |
| 36:BN:99:LEU:O     | 36:BN:102:ALA:HB3  | 2.21                     | 0.41              |
| 27:BA:1666:G:O3'   | 37:BO:6:THR:HG23   | 2.20                     | 0.41              |
| 39:BQ:58:PHE:CE1   | 39:BQ:61:GLY:HA3   | 2.56                     | 0.41              |
| 42:BT:129:ARG:HH11 | 42:BT:131:ALA:N    | 2.19                     | 0.41              |
| 42:BT:93:ARG:O     | 42:BT:94:ALA:C     | 2.57                     | 0.41              |
| 43:BU:85:LYS:CD    | 43:BU:117:GLN:HE22 | 2.33                     | 0.41              |
| 43:BU:22:LYS:HD3   | 43:BU:22:LYS:HA    | 1.92                     | 0.41              |
| 43:BU:52:ARG:HH11  | 43:BU:52:ARG:CG    | 2.33                     | 0.41              |
| 43:BU:65:ILE:C     | 43:BU:67:ALA:N     | 2.73                     | 0.41              |
| 44:BV:2:PHE:HE1    | 44:BV:13:ARG:HG3   | 1.85                     | 0.41              |
| 44:BV:21:ARG:HD3   | 44:BV:21:ARG:H     | 1.86                     | 0.41              |
| 44:BV:62:LEU:H     | 44:BV:62:LEU:CD2   | 2.21                     | 0.41              |
| 47:BY:15:VAL:HG12  | 47:BY:17:SER:H     | 1.86                     | 0.41              |
| 47:BY:97:ARG:O     | 47:BY:98:VAL:CB    | 2.68                     | 0.41              |
| 48:BZ:127:VAL:HG11 | 48:BZ:132:ILE:HG12 | 2.02                     | 0.41              |
| 48:BZ:63:GLY:O     | 48:BZ:64:GLN:O     | 2.38                     | 0.41              |
| 1:CA:1096:C:H2'    | 1:CA:1097:C:H6     | 1.83                     | 0.41              |
| 1:CA:1125:U:H2'    | 1:CA:1125:U:O2     | 2.19                     | 0.41              |
| 1:CA:15:G:N7       | 1:CA:1396:A:C4     | 2.88                     | 0.41              |
| 1:CA:414:A:C2      | 1:CA:415:A:H1'     | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:532:A:O2'    | 1:CA:533:A:H5'    | 2.21                     | 0.41              |
| 1:CA:575:G:H4'    | 1:CA:576:G:O5'    | 2.20                     | 0.41              |
| 1:CA:922:G:H4'    | 5:CE:20:GLN:HA    | 2.03                     | 0.41              |
| 2:CB:114:ARG:NH1  | 2:CB:118:LEU:HD21 | 2.35                     | 0.41              |
| 2:CB:26:PRO:C     | 2:CB:28:PHE:H     | 2.23                     | 0.41              |
| 3:CC:37:GLN:OE1   | 3:CC:37:GLN:HA    | 2.19                     | 0.41              |
| 4:CD:101:LEU:HD22 | 4:CD:138:TYR:HB3  | 2.02                     | 0.41              |
| 4:CD:128:VAL:CG1  | 4:CD:129:ASN:ND2  | 2.84                     | 0.41              |
| 4:CD:128:VAL:HG13 | 4:CD:129:ASN:ND2  | 2.36                     | 0.41              |
| 4:CD:147:ALA:HB2  | 4:CD:182:LYS:HB3  | 2.02                     | 0.41              |
| 4:CD:64:LEU:CD2   | 4:CD:93:PHE:HE1   | 2.34                     | 0.41              |
| 5:CE:33:VAL:HG12  | 5:CE:34:VAL:N     | 2.35                     | 0.41              |
| 2:CB:178:ARG:HH21 | 8:CH:68:ARG:HH12  | 1.69                     | 0.41              |
| 8:CH:78:GLN:O     | 8:CH:81:HIS:CE1   | 2.74                     | 0.41              |
| 12:CL:114:ARG:NH2 | 12:CL:121:LYS:HB2 | 2.34                     | 0.41              |
| 12:CL:56:ARG:HA   | 12:CL:62:GLU:HA   | 2.03                     | 0.41              |
| 15:CO:36:ILE:O    | 15:CO:40:SER:N    | 2.43                     | 0.41              |
| 15:CO:45:VAL:HG12 | 15:CO:46:HIS:N    | 2.36                     | 0.41              |
| 17:CQ:4:LYS:HG3   | 17:CQ:6:LEU:HD11  | 2.01                     | 0.41              |
| 19:CS:66:MET:O    | 19:CS:66:MET:HG3  | 2.20                     | 0.41              |
| 49:D0:30:VAL:CG1  | 49:D0:66:VAL:HG22 | 2.50                     | 0.41              |
| 51:D2:25:VAL:O    | 51:D2:29:LYS:HG2  | 2.20                     | 0.41              |
| 27:DA:458:G:H3'   | 56:D7:38:GLY:O    | 2.21                     | 0.41              |
| 27:DA:1336:A:C2   | 27:DA:1337:G:C5   | 3.08                     | 0.41              |
| 27:DA:1427:A:HO2' | 27:DA:1428:C:P    | 2.42                     | 0.41              |
| 27:DA:1502:C:H2'  | 27:DA:1502:C:O2   | 2.19                     | 0.41              |
| 27:DA:1567:A:H5'' | 30:DD:58:HIS:NE2  | 2.36                     | 0.41              |
| 27:DA:1844:C:H2'  | 27:DA:1845:G:H8   | 1.84                     | 0.41              |
| 27:DA:2048:G:C2'  | 27:DA:2049:G:O5'  | 2.69                     | 0.41              |
| 27:DA:2092:U:O2'  | 27:DA:2093:G:OP2  | 2.30                     | 0.41              |
| 27:DA:2277:G:C2'  | 27:DA:2278:A:H5'  | 2.51                     | 0.41              |
| 27:DA:230:U:H2'   | 27:DA:231:C:C6    | 2.53                     | 0.41              |
| 27:DA:2314:C:H2'  | 27:DA:2315:G:H8   | 1.84                     | 0.41              |
| 27:DA:2293:C:N3   | 27:DA:2340:G:C2   | 2.89                     | 0.41              |
| 27:DA:2467:C:C4   | 27:DA:2468:G:C2   | 3.09                     | 0.41              |
| 27:DA:2729:G:H2'  | 27:DA:2730:C:H6   | 1.85                     | 0.41              |
| 27:DA:2810:A:C8   | 27:DA:2811:G:C8   | 3.08                     | 0.41              |
| 27:DA:312:G:C5    | 27:DA:313:C:C5    | 3.09                     | 0.41              |
| 27:DA:416:C:C2    | 27:DA:417:C:C6    | 3.09                     | 0.41              |
| 27:DA:308:G:N2    | 27:DA:477:A:C8    | 2.89                     | 0.41              |
| 27:DA:574:C:H1'   | 27:DA:2055:C:C5   | 2.53                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:592:G:H21    | 57:D8:4:MET:CE    | 2.33                     | 0.41              |
| 27:DA:81:G:H21     | 47:DY:2:ARG:NH1   | 2.18                     | 0.41              |
| 27:DA:971:C:H2'    | 27:DA:972:G:H5'   | 2.02                     | 0.41              |
| 28:DB:94:C:H2'     | 28:DB:94:C:O2     | 2.20                     | 0.41              |
| 29:DC:56:GLN:OE1   | 29:DC:168:THR:CB  | 2.69                     | 0.41              |
| 29:DC:95:GLY:HA3   | 29:DC:99:ILE:HD12 | 2.02                     | 0.41              |
| 33:DG:173:LEU:HD22 | 33:DG:178:PHE:CE1 | 2.55                     | 0.41              |
| 34:DH:92:ILE:CG2   | 34:DH:93:GLY:H    | 2.22                     | 0.41              |
| 35:DI:126:TYR:O    | 35:DI:139:GLN:HA  | 2.20                     | 0.41              |
| 36:DN:27:ALA:CB    | 36:DN:106:MET:HE1 | 2.49                     | 0.41              |
| 37:DO:97:ARG:NE    | 37:DO:99:PHE:HE1  | 2.16                     | 0.41              |
| 38:DP:67:MET:HG3   | 38:DP:67:MET:O    | 2.21                     | 0.41              |
| 39:DQ:94:VAL:HG23  | 39:DQ:95:ALA:N    | 2.35                     | 0.41              |
| 42:DT:11:GLU:CD    | 42:DT:11:GLU:N    | 2.74                     | 0.41              |
| 42:DT:16:ARG:HH11  | 42:DT:16:ARG:HG3  | 1.84                     | 0.41              |
| 44:DV:19:LYS:HG2   | 44:DV:94:LEU:HB2  | 2.03                     | 0.41              |
| 45:DW:29:LEU:CD1   | 45:DW:51:LEU:HD11 | 2.50                     | 0.41              |
| 46:DX:47:PHE:HD2   | 46:DX:89:ILE:HG12 | 1.85                     | 0.41              |
| 47:DY:31:LEU:HA    | 47:DY:31:LEU:HD13 | 1.69                     | 0.41              |
| 1:AA:1064:G:H1'    | 1:AA:1066:C:C6    | 2.56                     | 0.41              |
| 1:AA:1088:G:C5     | 1:AA:1089:G:N7    | 2.89                     | 0.41              |
| 1:AA:123:C:N3      | 1:AA:238:G:N2     | 2.62                     | 0.41              |
| 1:AA:1327:C:H2'    | 1:AA:1328:C:C6    | 2.55                     | 0.41              |
| 1:AA:1339:A:H1'    | 24:AX:41:C:H1'    | 2.03                     | 0.41              |
| 1:AA:1508:G:C4     | 1:AA:1509:C:C5    | 3.08                     | 0.41              |
| 1:AA:189(I):G:C2'  | 1:AA:189(J):G:H8  | 2.34                     | 0.41              |
| 1:AA:223:U:H2'     | 1:AA:224:C:O4'    | 2.20                     | 0.41              |
| 1:AA:373:A:C2      | 1:AA:374:A:C8     | 3.09                     | 0.41              |
| 1:AA:927:G:C2'     | 1:AA:928:G:H5'    | 2.50                     | 0.41              |
| 2:AB:210:SER:O     | 2:AB:211:ILE:C    | 2.59                     | 0.41              |
| 3:AC:184:TYR:HA    | 3:AC:200:ALA:O    | 2.20                     | 0.41              |
| 6:AF:24:GLU:CG     | 6:AF:25:ILE:H     | 2.33                     | 0.41              |
| 7:AG:115:ARG:O     | 7:AG:118:VAL:HG22 | 2.21                     | 0.41              |
| 7:AG:26:PHE:CE2    | 7:AG:30:ILE:HD11  | 2.55                     | 0.41              |
| 7:AG:27:ILE:HG22   | 7:AG:39:ALA:HB1   | 2.02                     | 0.41              |
| 7:AG:63:LYS:HZ1    | 7:AG:67:GLU:HB2   | 1.86                     | 0.41              |
| 7:AG:94:ARG:O      | 7:AG:97:GLN:N     | 2.53                     | 0.41              |
| 11:AK:85:ARG:O     | 11:AK:86:GLY:O    | 2.39                     | 0.41              |
| 12:AL:25:LYS:HE2   | 12:AL:30:ARG:NH2  | 2.36                     | 0.41              |
| 12:AL:88:LYS:HE2   | 12:AL:88:LYS:HB2  | 1.79                     | 0.41              |
| 13:AM:40:ASN:C     | 13:AM:42:ALA:H    | 2.24                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:45:VAL:C     | 13:AM:47:ASP:H     | 2.23                     | 0.41              |
| 14:AN:40:CYS:C     | 14:AN:42:ILE:H     | 2.24                     | 0.41              |
| 16:AP:19:ILE:CD1   | 16:AP:73:LEU:HD12  | 2.48                     | 0.41              |
| 17:AQ:68:ARG:H     | 17:AQ:70:ARG:HH12  | 1.67                     | 0.41              |
| 18:AR:37:VAL:CG2   | 18:AR:38:GLU:H     | 2.22                     | 0.41              |
| 55:B6:9:LEU:HD21   | 55:B6:26:ASN:HD22  | 1.85                     | 0.41              |
| 27:BA:105:C:O2     | 27:BA:105:C:C2'    | 2.60                     | 0.41              |
| 27:BA:1028:A:H61   | 27:BA:1125:G:H2'   | 1.81                     | 0.41              |
| 27:BA:729:G:C4     | 27:BA:1775:U:O2    | 2.74                     | 0.41              |
| 27:BA:1826:G:OP1   | 30:BD:224:ALA:N    | 2.47                     | 0.41              |
| 27:BA:1846:G:H5''  | 27:BA:1847:A:OP2   | 2.20                     | 0.41              |
| 27:BA:1905:C:H1'   | 27:BA:1928:A:H2    | 1.85                     | 0.41              |
| 27:BA:1936:A:C3'   | 27:BA:1937:A:H5''  | 2.43                     | 0.41              |
| 27:BA:2010:G:H5''  | 45:BW:42:ARG:HB3   | 2.02                     | 0.41              |
| 27:BA:2065:C:H1'   | 27:BA:2449:U:O2    | 2.20                     | 0.41              |
| 27:BA:2171:A:H4'   | 27:BA:2172:U:C5'   | 2.47                     | 0.41              |
| 27:BA:258:G:H2'    | 27:BA:259:G:C8     | 2.52                     | 0.41              |
| 27:BA:237:C:N3     | 27:BA:261:G:C2     | 2.89                     | 0.41              |
| 27:BA:2703:C:H2'   | 27:BA:2704:C:H6    | 1.85                     | 0.41              |
| 27:BA:2788:C:H4'   | 27:BA:2810:A:C4'   | 2.51                     | 0.41              |
| 27:BA:2843:G:C5    | 27:BA:2844:G:C8    | 3.09                     | 0.41              |
| 27:BA:914:C:C2'    | 27:BA:915:C:O5'    | 2.68                     | 0.41              |
| 27:BA:970:C:H2'    | 27:BA:971:C:C6     | 2.56                     | 0.41              |
| 28:BB:58:A:C5      | 28:BB:59:A:C8      | 3.09                     | 0.41              |
| 29:BC:100:ILE:HG22 | 29:BC:101:GLN:CG   | 2.46                     | 0.41              |
| 30:BD:106:ILE:CD1  | 30:BD:157:ARG:HA   | 2.51                     | 0.41              |
| 30:BD:165:ILE:O    | 30:BD:166:GLN:NE2  | 2.54                     | 0.41              |
| 31:BE:102:VAL:HG12 | 31:BE:200:GLU:HA   | 2.03                     | 0.41              |
| 32:BF:157:VAL:HG21 | 32:BF:181:LEU:HD13 | 2.02                     | 0.41              |
| 33:BG:121:ASN:HA   | 33:BG:122:PRO:HD2  | 1.79                     | 0.41              |
| 33:BG:71:THR:OG1   | 33:BG:89:GLY:HA3   | 2.20                     | 0.41              |
| 34:BH:23:ARG:O     | 34:BH:24:VAL:HG13  | 2.21                     | 0.41              |
| 36:BN:4:TYR:HE2    | 43:BU:61:TRP:HE1   | 1.65                     | 0.41              |
| 38:BP:101:VAL:CG1  | 38:BP:106:LEU:HD23 | 2.51                     | 0.41              |
| 39:BQ:31:ASP:O     | 39:BQ:133:ARG:O    | 2.38                     | 0.41              |
| 41:BS:68:GLN:O     | 41:BS:71:ARG:HB2   | 2.21                     | 0.41              |
| 42:BT:28:VAL:HG12  | 42:BT:29:ARG:NE    | 2.36                     | 0.41              |
| 37:BO:122:LEU:HD23 | 42:BT:43:GLN:NE2   | 2.36                     | 0.41              |
| 27:BA:18:C:H5''    | 43:BU:24:TYR:O     | 2.20                     | 0.41              |
| 44:BV:35:LEU:N     | 44:BV:35:LEU:CD2   | 2.83                     | 0.41              |
| 46:BX:14:SER:O     | 46:BX:15:GLU:C     | 2.59                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:BZ:46:VAL:HG12 | 48:BZ:50:ALA:HB3  | 2.03                     | 0.41              |
| 48:BZ:67:PRO:O    | 48:BZ:68:THR:HG23 | 2.21                     | 0.41              |
| 1:CA:1058:G:C5    | 1:CA:1059:C:C4    | 3.09                     | 0.41              |
| 1:CA:1076:C:H2'   | 1:CA:1077:G:H8    | 1.86                     | 0.41              |
| 1:CA:1316:G:O6    | 19:CS:5:LEU:HD22  | 2.20                     | 0.41              |
| 1:CA:133:U:H1'    | 1:CA:230:G:H21    | 1.84                     | 0.41              |
| 1:CA:1350:A:H2'   | 1:CA:1351:U:C6    | 2.55                     | 0.41              |
| 1:CA:1407:C:O2    | 27:DA:1912:A:C2   | 2.68                     | 0.41              |
| 1:CA:1412:C:H2'   | 1:CA:1413:A:H8    | 1.79                     | 0.41              |
| 1:CA:1494:G:H8    | 1:CA:1494:G:OP2   | 2.02                     | 0.41              |
| 1:CA:217:C:O2'    | 1:CA:218:C:P      | 2.79                     | 0.41              |
| 1:CA:407:G:N2     | 1:CA:436:C:C2     | 2.89                     | 0.41              |
| 1:CA:594:G:C2'    | 1:CA:595:G:H5'    | 2.51                     | 0.41              |
| 1:CA:658:G:H2'    | 1:CA:659:U:C6     | 2.55                     | 0.41              |
| 1:CA:854:G:H3'    | 1:CA:871:U:O4     | 2.21                     | 0.41              |
| 1:CA:865:A:C2     | 1:CA:866:C:O2     | 2.74                     | 0.41              |
| 1:CA:894:G:C6     | 1:CA:895:G:C6     | 3.09                     | 0.41              |
| 1:CA:932:C:C2'    | 1:CA:932:C:O2     | 2.66                     | 0.41              |
| 2:CB:57:PHE:CE2   | 2:CB:185:ILE:HD11 | 2.56                     | 0.41              |
| 2:CB:87:ARG:HE    | 2:CB:233:SER:HB2  | 1.86                     | 0.41              |
| 3:CC:68:VAL:HG12  | 3:CC:70:VAL:CG2   | 2.51                     | 0.41              |
| 3:CC:90:GLU:O     | 3:CC:93:LYS:HB3   | 2.21                     | 0.41              |
| 3:CC:91:LEU:O     | 3:CC:94:LEU:HD12  | 2.21                     | 0.41              |
| 4:CD:114:ARG:O    | 4:CD:117:ALA:N    | 2.53                     | 0.41              |
| 4:CD:11:LEU:HD23  | 4:CD:11:LEU:H     | 1.85                     | 0.41              |
| 4:CD:8:VAL:O      | 4:CD:10:ARG:N     | 2.43                     | 0.41              |
| 4:CD:91:SER:O     | 4:CD:92:VAL:C     | 2.59                     | 0.41              |
| 5:CE:146:ALA:O    | 5:CE:147:ASP:C    | 2.58                     | 0.41              |
| 5:CE:6:PHE:N      | 5:CE:6:PHE:CD1    | 2.88                     | 0.41              |
| 7:CG:134:ALA:O    | 7:CG:137:LYS:N    | 2.54                     | 0.41              |
| 7:CG:15:ASP:OD2   | 7:CG:16:LEU:N     | 2.47                     | 0.41              |
| 12:CL:30:ARG:HE   | 12:CL:30:ARG:HA   | 1.84                     | 0.41              |
| 14:CN:40:CYS:SG   | 14:CN:43:CYS:SG   | 3.09                     | 0.41              |
| 20:CT:30:LYS:HZ2  | 20:CT:80:ARG:NH2  | 2.16                     | 0.41              |
| 26:CZ:6:5OH:CS    | 26:CZ:6:5OH:N     | 2.83                     | 0.41              |
| 51:D2:29:LYS:CD   | 51:D2:57:ILE:HD12 | 2.51                     | 0.41              |
| 55:D6:18:ARG:HB2  | 55:D6:19:ARG:H    | 1.78                     | 0.41              |
| 55:D6:42:TRP:HA   | 55:D6:42:TRP:CE3  | 2.55                     | 0.41              |
| 27:DA:1031:G:C4'  | 58:D9:6:SER:OG    | 2.66                     | 0.41              |
| 27:DA:1152:C:C1'  | 43:DU:77:SER:HB2  | 2.50                     | 0.41              |
| 27:DA:1157:G:H2'  | 27:DA:1158:C:C5   | 2.53                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:1236:G:O2'   | 27:DA:1237:A:P    | 2.78                     | 0.41              |
| 27:DA:1294:U:H5''  | 27:DA:1295:C:OP2  | 2.21                     | 0.41              |
| 27:DA:1494:A:HO2'  | 27:DA:1495:A:H5'' | 1.77                     | 0.41              |
| 27:DA:1615:C:O2'   | 27:DA:1616:A:P    | 2.79                     | 0.41              |
| 27:DA:1788:C:C2'   | 27:DA:1789:A:H5'  | 2.50                     | 0.41              |
| 27:DA:1792:G:H8    | 27:DA:1792:G:O5'  | 2.03                     | 0.41              |
| 27:DA:1843:C:H6    | 27:DA:1843:C:O5'  | 2.04                     | 0.41              |
| 27:DA:1899:G:H21   | 27:DA:1902:C:N4   | 2.18                     | 0.41              |
| 27:DA:1906:G:C2    | 27:DA:1907:G:C5   | 3.09                     | 0.41              |
| 27:DA:1946:U:C2'   | 27:DA:1947:C:H6   | 2.27                     | 0.41              |
| 27:DA:2244:U:O5'   | 27:DA:2244:U:H6   | 2.04                     | 0.41              |
| 27:DA:2321:G:N3    | 27:DA:2321:G:H2'  | 2.34                     | 0.41              |
| 27:DA:2335:A:O2'   | 27:DA:2336:A:H5'' | 2.20                     | 0.41              |
| 27:DA:2468:G:HO2'  | 27:DA:2469:A:P    | 2.44                     | 0.41              |
| 27:DA:2569:G:H2'   | 27:DA:2570:G:H5'  | 2.02                     | 0.41              |
| 27:DA:2691:C:C6    | 27:DA:2691:C:H5'  | 2.56                     | 0.41              |
| 27:DA:2826:A:H3'   | 27:DA:2827:C:H6   | 1.85                     | 0.41              |
| 27:DA:2835:A:C6    | 27:DA:2879:C:C6   | 3.09                     | 0.41              |
| 27:DA:2840:C:O2'   | 27:DA:2841:C:H5'  | 2.21                     | 0.41              |
| 27:DA:319:C:H2'    | 27:DA:320:A:O4'   | 2.20                     | 0.41              |
| 27:DA:370:G:O2'    | 27:DA:371:A:OP1   | 2.31                     | 0.41              |
| 27:DA:583:G:C5     | 27:DA:584:C:C5    | 3.09                     | 0.41              |
| 27:DA:61:G:O5'     | 27:DA:61:G:H8     | 2.02                     | 0.41              |
| 27:DA:930:U:H4'    | 27:DA:931:G:N3    | 2.35                     | 0.41              |
| 28:DB:105:A:H2'    | 28:DB:106:G:O4'   | 2.20                     | 0.41              |
| 29:DC:51:PRO:HB3   | 29:DC:203:GLY:O   | 2.20                     | 0.41              |
| 27:DA:1902:C:OP1   | 30:DD:242:ARG:HD3 | 2.21                     | 0.41              |
| 31:DE:57:LYS:C     | 31:DE:59:VAL:N    | 2.73                     | 0.41              |
| 31:DE:52:LEU:CD2   | 31:DE:76:ARG:HD3  | 2.50                     | 0.41              |
| 32:DF:156:LEU:HD12 | 32:DF:156:LEU:HA  | 1.79                     | 0.41              |
| 32:DF:2:LYS:CD     | 32:DF:2:LYS:N     | 2.69                     | 0.41              |
| 33:DG:130:ASN:HB3  | 33:DG:160:VAL:HA  | 2.02                     | 0.41              |
| 33:DG:129:GLY:O    | 33:DG:161:THR:CB  | 2.68                     | 0.41              |
| 33:DG:165:THR:OG1  | 33:DG:168:GLU:HB2 | 2.20                     | 0.41              |
| 33:DG:39:ILE:HG23  | 33:DG:92:VAL:CG1  | 2.40                     | 0.41              |
| 35:DI:9:LEU:O      | 35:DI:12:LEU:O    | 2.39                     | 0.41              |
| 35:DI:45:LYS:O     | 35:DI:48:GLU:CB   | 2.69                     | 0.41              |
| 35:DI:69:LYS:O     | 35:DI:73:GLU:CB   | 2.69                     | 0.41              |
| 36:DN:89:LYS:HA    | 36:DN:89:LYS:HD2  | 1.77                     | 0.41              |
| 37:DO:86:ILE:H     | 37:DO:86:ILE:CD1  | 2.28                     | 0.41              |
| 27:DA:1285:G:O3'   | 40:DR:105:ARG:NH1 | 2.54                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:DR:12:ARG:O     | 40:DR:17:ARG:NH2  | 2.54                     | 0.41              |
| 41:DS:25:ARG:NH1   | 41:DS:40:ILE:HB   | 2.35                     | 0.41              |
| 42:DT:50:ILE:CG2   | 42:DT:100:TYR:HA  | 2.49                     | 0.41              |
| 42:DT:13:ARG:NH1   | 42:DT:13:ARG:HA   | 2.36                     | 0.41              |
| 37:DO:101:PRO:CG   | 42:DT:67:SER:OG   | 2.65                     | 0.41              |
| 45:DW:12:ILE:CG1   | 45:DW:42:ARG:NH1  | 2.84                     | 0.41              |
| 47:DY:18:GLY:C     | 47:DY:20:TYR:N    | 2.74                     | 0.41              |
| 48:DZ:51:SER:HB3   | 48:DZ:53:HIS:HD2  | 1.86                     | 0.41              |
| 48:DZ:71:ARG:HD3   | 48:DZ:71:ARG:HA   | 1.62                     | 0.41              |
| 1:AA:1045:C:C6     | 1:AA:1045:C:C3'   | 3.04                     | 0.41              |
| 1:AA:1217:C:O2'    | 1:AA:1218:C:H5'   | 2.21                     | 0.41              |
| 1:AA:1239:A:N3     | 1:AA:1241:G:N1    | 2.69                     | 0.41              |
| 1:AA:1256:A:C5'    | 1:AA:1257:U:OP1   | 2.62                     | 0.41              |
| 1:AA:1365:G:O2'    | 1:AA:1366:C:C5'   | 2.69                     | 0.41              |
| 1:AA:336:C:C1'     | 1:AA:1468:A:H2    | 2.34                     | 0.41              |
| 1:AA:1499:A:C1'    | 1:AA:1520:G:H5'   | 2.49                     | 0.41              |
| 1:AA:22:G:O2'      | 1:AA:23:C:H5'     | 2.21                     | 0.41              |
| 1:AA:255:G:C4      | 1:AA:256:U:C5     | 3.09                     | 0.41              |
| 1:AA:289:G:C2      | 1:AA:312:C:O2     | 2.73                     | 0.41              |
| 1:AA:460:G:N1      | 1:AA:470:C:H5''   | 2.34                     | 0.41              |
| 1:AA:747:C:C2'     | 1:AA:748:C:O5'    | 2.68                     | 0.41              |
| 1:AA:837:G:C2      | 1:AA:850:U:O2     | 2.74                     | 0.41              |
| 1:AA:969:A:C2      | 1:AA:970:C:C2     | 3.08                     | 0.41              |
| 3:AC:54:ARG:O      | 3:AC:55:VAL:HG23  | 2.21                     | 0.41              |
| 4:AD:3:ARG:HB3     | 4:AD:118:ARG:NH1  | 2.33                     | 0.41              |
| 5:AE:34:VAL:CG1    | 5:AE:35:GLY:N     | 2.83                     | 0.41              |
| 5:AE:53:LEU:H      | 5:AE:53:LEU:HD12  | 1.85                     | 0.41              |
| 1:AA:19:C:H5''     | 5:AE:86:ALA:HB3   | 2.03                     | 0.41              |
| 7:AG:40:ALA:O      | 7:AG:41:ARG:C     | 2.59                     | 0.41              |
| 8:AH:2:LEU:HD13    | 8:AH:3:THR:N      | 2.36                     | 0.41              |
| 8:AH:84:ARG:HG3    | 8:AH:85:ARG:N     | 2.35                     | 0.41              |
| 8:AH:97:VAL:HG22   | 8:AH:98:LYS:N     | 2.36                     | 0.41              |
| 1:AA:1152:A:H3'    | 10:AJ:13:HIS:CD2  | 2.56                     | 0.41              |
| 10:AJ:67:THR:O     | 10:AJ:67:THR:HG23 | 2.20                     | 0.41              |
| 10:AJ:78:ASN:ND2   | 10:AJ:81:THR:OG1  | 2.54                     | 0.41              |
| 11:AK:51:LYS:HB3   | 11:AK:51:LYS:HZ3  | 1.86                     | 0.41              |
| 12:AL:24:LEU:N     | 12:AL:24:LEU:HD22 | 2.35                     | 0.41              |
| 13:AM:108:ARG:NH1  | 13:AM:111:LYS:O   | 2.54                     | 0.41              |
| 13:AM:117:VAL:HG12 | 13:AM:118:ALA:O   | 2.21                     | 0.41              |
| 13:AM:3:ARG:HA     | 13:AM:8:GLU:O     | 2.20                     | 0.41              |
| 14:AN:40:CYS:C     | 14:AN:42:ILE:N    | 2.74                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 16:AP:3:LYS:O     | 16:AP:21:VAL:HA     | 2.21                     | 0.41              |
| 19:AS:38:SER:O    | 19:AS:70:LYS:HD2    | 2.21                     | 0.41              |
| 21:AU:9:ARG:HD3   | 21:AU:22:ARG:HD2    | 2.02                     | 0.41              |
| 24:AX:4:G:C5      | 24:AX:70:G:C6       | 3.09                     | 0.41              |
| 51:B2:19:VAL:HG12 | 51:B2:20:GLU:N      | 2.35                     | 0.41              |
| 54:B5:57:VAL:C    | 54:B5:58:LEU:HD23   | 2.41                     | 0.41              |
| 55:B6:19:ARG:CG   | 55:B6:20:ASN:H      | 2.22                     | 0.41              |
| 55:B6:25:LYS:HD2  | 55:B6:27:LYS:HZ3    | 1.84                     | 0.41              |
| 55:B6:41:PRO:CD   | 55:B6:46:HIS:HB3    | 2.46                     | 0.41              |
| 55:B6:47:THR:HB   | 55:B6:48:VAL:H      | 1.59                     | 0.41              |
| 55:B6:9:LEU:HD13  | 55:B6:28:ARG:CG     | 2.51                     | 0.41              |
| 27:BA:1139:G:N3   | 27:BA:1143:A:H2     | 2.19                     | 0.41              |
| 27:BA:1204:A:H2   | 27:BA:1241:A:N1     | 2.18                     | 0.41              |
| 27:BA:1450:G:C2'  | 27:BA:1450(A):C:C5' | 2.98                     | 0.41              |
| 27:BA:1593:G:C3'  | 27:BA:1594:G:H8     | 2.33                     | 0.41              |
| 27:BA:1685:C:C3'  | 27:BA:1686:C:H5''   | 2.51                     | 0.41              |
| 27:BA:1806:C:C2'  | 27:BA:1807:G:H5'    | 2.50                     | 0.41              |
| 27:BA:1975:G:H2'  | 27:BA:1976:U:H5'    | 2.03                     | 0.41              |
| 27:BA:2109:U:C4   | 27:BA:2110:G:O6     | 2.74                     | 0.41              |
| 27:BA:2136:C:N4   | 27:BA:2155:G:H1     | 2.18                     | 0.41              |
| 25:AY:75:A:H1'    | 27:BA:2421:G:N2     | 2.36                     | 0.41              |
| 27:BA:2425:A:O4'  | 27:BA:2427:C:C2     | 2.74                     | 0.41              |
| 27:BA:2468:G:H22  | 27:BA:2481:G:C2'    | 2.34                     | 0.41              |
| 27:BA:2487:G:O2'  | 27:BA:2488:A:H5'    | 2.21                     | 0.41              |
| 27:BA:2536:G:C5   | 27:BA:2537:U:C5     | 3.08                     | 0.41              |
| 27:BA:2694:G:H8   | 27:BA:2694:G:C5'    | 2.23                     | 0.41              |
| 27:BA:2641:G:N1   | 27:BA:2774:C:C4     | 2.89                     | 0.41              |
| 27:BA:301:G:O2'   | 27:BA:302:C:P       | 2.78                     | 0.41              |
| 27:BA:397:G:H2'   | 27:BA:398:G:C8      | 2.56                     | 0.41              |
| 27:BA:501:A:H2'   | 27:BA:502:A:C8      | 2.55                     | 0.41              |
| 27:BA:523:C:H6    | 27:BA:523:C:O5'     | 2.03                     | 0.41              |
| 27:BA:604:G:C6    | 27:BA:605:C:C4      | 3.08                     | 0.41              |
| 27:BA:603:A:H4'   | 27:BA:604:G:OP1     | 2.21                     | 0.41              |
| 27:BA:607:U:C5    | 27:BA:620:G:C5      | 3.09                     | 0.41              |
| 27:BA:700:G:C2    | 27:BA:701:G:C4      | 3.08                     | 0.41              |
| 27:BA:722:A:N1    | 27:BA:723:G:C4      | 2.88                     | 0.41              |
| 27:BA:723:G:C6    | 27:BA:724:U:N3      | 2.89                     | 0.41              |
| 27:BA:726:G:O2'   | 27:BA:727:A:P       | 2.78                     | 0.41              |
| 27:BA:778:G:C5    | 27:BA:779:U:C4      | 3.09                     | 0.41              |
| 27:BA:888:C:C3'   | 27:BA:889:C:C5'     | 2.99                     | 0.41              |
| 27:BA:873:G:H1    | 27:BA:904:C:H42     | 1.69                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BB:31:C:H41    | 41:BS:32:LEU:HD13  | 1.84                     | 0.41              |
| 28:BB:40:U:O2     | 28:BB:43:C:H5''    | 2.21                     | 0.41              |
| 28:BB:40:U:H1'    | 28:BB:45:A:H61     | 1.85                     | 0.41              |
| 28:BB:61:G:N2     | 28:BB:62:C:C2      | 2.88                     | 0.41              |
| 28:BB:64:C:C4     | 28:BB:65:C:C5      | 3.08                     | 0.41              |
| 30:BD:240:ALA:HA  | 30:BD:241:PRO:HD3  | 1.48                     | 0.41              |
| 27:BA:2228:G:P    | 30:BD:261:LYS:HZ1  | 2.43                     | 0.41              |
| 30:BD:27:THR:HG21 | 30:BD:83:GLU:CA    | 2.51                     | 0.41              |
| 31:BE:54:GLN:HB2  | 31:BE:55:ASN:H     | 1.53                     | 0.41              |
| 32:BF:149:ASP:OD2 | 32:BF:149:ASP:N    | 2.54                     | 0.41              |
| 32:BF:177:ALA:O   | 32:BF:180:GLY:N    | 2.43                     | 0.41              |
| 33:BG:7:LEU:HD23  | 33:BG:10:LYS:HB2   | 2.02                     | 0.41              |
| 33:BG:11:TYR:HE2  | 33:BG:12:TYR:CE2   | 2.39                     | 0.41              |
| 34:BH:19:VAL:CG2  | 34:BH:44:VAL:HG13  | 2.51                     | 0.41              |
| 34:BH:54:ARG:CG   | 34:BH:54:ARG:O     | 2.69                     | 0.41              |
| 35:BI:19:VAL:HG22 | 35:BI:20:ASP:N     | 2.36                     | 0.41              |
| 37:BO:98:VAL:HG13 | 37:BO:118:ALA:HA   | 2.03                     | 0.41              |
| 37:BO:3:GLN:O     | 37:BO:4:PRO:C      | 2.58                     | 0.41              |
| 38:BP:83:VAL:CG1  | 38:BP:112:LEU:HD21 | 2.51                     | 0.41              |
| 39:BQ:16:ARG:CG   | 39:BQ:17:LEU:H     | 2.32                     | 0.41              |
| 39:BQ:70:PRO:HA   | 39:BQ:94:VAL:C     | 2.41                     | 0.41              |
| 42:BT:28:VAL:O    | 42:BT:86:ILE:O     | 2.39                     | 0.41              |
| 44:BV:38:LEU:C    | 44:BV:39:LEU:HD13  | 2.41                     | 0.41              |
| 45:BW:34:ASN:HA   | 45:BW:34:ASN:HD22  | 1.70                     | 0.41              |
| 47:BY:84:ARG:NH1  | 47:BY:97:ARG:HA    | 2.35                     | 0.41              |
| 48:BZ:38:VAL:HG23 | 48:BZ:43:PHE:HB2   | 2.01                     | 0.41              |
| 48:BZ:43:PHE:CD1  | 48:BZ:44:ASP:N     | 2.88                     | 0.41              |
| 1:CA:1065:U:C5    | 1:CA:1190:G:H1'    | 2.55                     | 0.41              |
| 1:CA:1480:G:C4    | 1:CA:1481:U:C6     | 3.09                     | 0.41              |
| 1:CA:27:G:C6      | 1:CA:28:G:C5       | 3.09                     | 0.41              |
| 1:CA:452:A:C6     | 1:CA:453:A:C5      | 3.09                     | 0.41              |
| 1:CA:485:G:O2'    | 1:CA:486:U:P       | 2.79                     | 0.41              |
| 1:CA:504:C:N3     | 1:CA:542:G:C2      | 2.89                     | 0.41              |
| 1:CA:610:G:O5'    | 1:CA:610:G:C8      | 2.74                     | 0.41              |
| 1:CA:687:A:N1     | 1:CA:700:G:O2'     | 2.49                     | 0.41              |
| 3:CC:113:ALA:O    | 3:CC:115:LEU:N     | 2.53                     | 0.41              |
| 3:CC:130:VAL:HG21 | 3:CC:157:ILE:HG23  | 2.03                     | 0.41              |
| 3:CC:50:ALA:HB2   | 3:CC:75:VAL:HG11   | 2.03                     | 0.41              |
| 4:CD:162:LEU:HD23 | 4:CD:162:LEU:HA    | 1.88                     | 0.41              |
| 4:CD:80:GLU:C     | 4:CD:84:LYS:HE2    | 2.40                     | 0.41              |
| 5:CE:40:ARG:HH11  | 5:CE:40:ARG:HG2    | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:CG:142:GLU:OE2  | 7:CG:142:GLU:HA   | 2.21                     | 0.41              |
| 8:CH:44:PHE:HD1   | 8:CH:79:VAL:CG1   | 2.34                     | 0.41              |
| 11:CK:86:GLY:C    | 11:CK:87:THR:O    | 2.57                     | 0.41              |
| 13:CM:14:ARG:N    | 13:CM:44:ARG:HH11 | 2.18                     | 0.41              |
| 13:CM:31:LYS:HA   | 13:CM:34:LEU:HB2  | 2.03                     | 0.41              |
| 15:CO:58:MET:HB3  | 15:CO:58:MET:HE3  | 1.90                     | 0.41              |
| 18:CR:22:VAL:O    | 18:CR:26:LEU:HG   | 2.20                     | 0.41              |
| 50:D1:71:TYR:CD1  | 50:D1:71:TYR:N    | 2.89                     | 0.41              |
| 50:D1:80:LEU:HD22 | 50:D1:82:LEU:CD1  | 2.50                     | 0.41              |
| 50:D1:94:LEU:O    | 50:D1:96:LYS:N    | 2.54                     | 0.41              |
| 51:D2:16:LEU:O    | 51:D2:17:SER:O    | 2.39                     | 0.41              |
| 51:D2:19:VAL:C    | 51:D2:21:LEU:N    | 2.74                     | 0.41              |
| 52:D3:19:GLN:HE22 | 52:D3:52:HIS:CE1  | 2.39                     | 0.41              |
| 55:D6:16:CYS:O    | 55:D6:18:ARG:NH2  | 2.54                     | 0.41              |
| 27:DA:1034:G:C5'  | 58:D9:18:ARG:HD2  | 2.36                     | 0.41              |
| 27:DA:2478:A:C5'  | 58:D9:31:LYS:NZ   | 2.82                     | 0.41              |
| 27:DA:1169:G:H1   | 27:DA:1180:C:H42  | 1.69                     | 0.41              |
| 27:DA:118:A:O2'   | 27:DA:178:G:H5'   | 2.20                     | 0.41              |
| 27:DA:1231:G:N1   | 27:DA:1232:G:C6   | 2.89                     | 0.41              |
| 27:DA:1313:U:H3'  | 27:DA:1314:C:H5'  | 2.03                     | 0.41              |
| 27:DA:1341:U:H3'  | 27:DA:1397:U:O2   | 2.20                     | 0.41              |
| 27:DA:1457:A:O2'  | 27:DA:1459:G:H8   | 2.02                     | 0.41              |
| 27:DA:1721:G:H2'  | 27:DA:1741:A:H62  | 1.86                     | 0.41              |
| 27:DA:1779:U:H5   | 27:DA:1784:A:C8   | 2.39                     | 0.41              |
| 27:DA:2228:G:C6   | 27:DA:2229:C:C4   | 3.09                     | 0.41              |
| 27:DA:2280:G:N7   | 49:D0:14:ARG:NH1  | 2.69                     | 0.41              |
| 27:DA:2415:G:H2'  | 27:DA:2416:C:H6   | 1.81                     | 0.41              |
| 27:DA:2545:G:N3   | 27:DA:2545:G:H2'  | 2.35                     | 0.41              |
| 27:DA:2668:G:C2'  | 27:DA:2669:G:H5'  | 2.51                     | 0.41              |
| 27:DA:412:A:OP1   | 27:DA:413:C:H5    | 2.04                     | 0.41              |
| 27:DA:700:G:H2'   | 27:DA:701:G:O4'   | 2.21                     | 0.41              |
| 27:DA:859:G:H21   | 27:DA:916:G:C2'   | 2.33                     | 0.41              |
| 27:DA:921:G:C6    | 27:DA:922:U:C4    | 3.09                     | 0.41              |
| 28:DB:24:G:O2'    | 28:DB:25:A:P      | 2.78                     | 0.41              |
| 30:DD:57:GLY:HA2  | 30:DD:214:TRP:O   | 2.20                     | 0.41              |
| 31:DE:154:LYS:HA  | 31:DE:154:LYS:HE3 | 2.01                     | 0.41              |
| 31:DE:54:GLN:HA   | 31:DE:72:VAL:HG12 | 2.02                     | 0.41              |
| 33:DG:154:GLY:O   | 33:DG:155:MET:HB3 | 2.21                     | 0.41              |
| 36:DN:70:LYS:HG2  | 36:DN:87:LEU:CD1  | 2.19                     | 0.41              |
| 40:DR:10:LEU:HD23 | 40:DR:17:ARG:HD2  | 2.02                     | 0.41              |
| 40:DR:20:LEU:HD12 | 40:DR:20:LEU:C    | 2.41                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 41:DS:82:ILE:CG2  | 41:DS:83:LYS:H      | 2.33                     | 0.41              |
| 42:DT:118:ARG:O   | 42:DT:119:LYS:C     | 2.59                     | 0.41              |
| 46:DX:11:PRO:O    | 46:DX:12:VAL:C      | 2.59                     | 0.41              |
| 27:DA:64:A:C6     | 46:DX:66:LEU:HD13   | 2.56                     | 0.41              |
| 47:DY:26:LYS:CG   | 47:DY:27:VAL:N      | 2.83                     | 0.41              |
| 47:DY:39:VAL:CG1  | 47:DY:40:GLU:N      | 2.63                     | 0.41              |
| 48:DZ:99:VAL:HA   | 48:DZ:100:PRO:HD3   | 1.90                     | 0.41              |
| 1:AA:1070:U:H2'   | 1:AA:1071:C:H6      | 1.80                     | 0.41              |
| 1:AA:1077:G:C8    | 1:AA:1077:G:H3'     | 2.56                     | 0.41              |
| 1:AA:1152:A:O2'   | 1:AA:1153:C:P       | 2.79                     | 0.41              |
| 1:AA:1399:C:C2    | 1:AA:1401:G:C6      | 3.09                     | 0.41              |
| 1:AA:162:A:OP2    | 1:AA:163:C:C4       | 2.74                     | 0.41              |
| 1:AA:295:C:C4     | 1:AA:296:U:C5       | 3.08                     | 0.41              |
| 1:AA:453:A:C6     | 1:AA:454:C:N4       | 2.88                     | 0.41              |
| 1:AA:721:G:H4'    | 1:AA:722:A:C5'      | 2.48                     | 0.41              |
| 1:AA:755:G:C6     | 1:AA:756:C:C4       | 3.09                     | 0.41              |
| 1:AA:579:G:N1     | 1:AA:763:G:C6       | 2.89                     | 0.41              |
| 1:AA:782:A:N1     | 1:AA:801:U:N1       | 2.68                     | 0.41              |
| 1:AA:852:G:C2'    | 1:AA:853:G:O5'      | 2.69                     | 0.41              |
| 1:AA:864:A:H3'    | 1:AA:865:A:C8       | 2.56                     | 0.41              |
| 1:AA:92:C:H2'     | 1:AA:93:G:C8        | 2.56                     | 0.41              |
| 2:AB:178:ARG:C    | 2:AB:180:LEU:N      | 2.73                     | 0.41              |
| 3:AC:33:LEU:O     | 3:AC:36:ASP:CB      | 2.68                     | 0.41              |
| 1:AA:1191:A:OP2   | 3:AC:3:ASN:ND2      | 2.54                     | 0.41              |
| 3:AC:62:ASP:O     | 3:AC:98:ASN:CB      | 2.68                     | 0.41              |
| 10:AJ:45:ARG:HB3  | 10:AJ:47:PHE:CZ     | 2.56                     | 0.41              |
| 11:AK:24:SER:HB3  | 11:AK:25:TYR:H      | 1.49                     | 0.41              |
| 12:AL:43:LYS:N    | 12:AL:89:ASP:O      | 2.53                     | 0.41              |
| 14:AN:26:ARG:CG   | 14:AN:27:CYS:H      | 2.17                     | 0.41              |
| 16:AP:44:THR:O    | 16:AP:45:THR:CB     | 2.69                     | 0.41              |
| 17:AQ:16:GLN:O    | 17:AQ:18:THR:N      | 2.54                     | 0.41              |
| 18:AR:85:LEU:HD12 | 18:AR:85:LEU:HA     | 1.75                     | 0.41              |
| 20:AT:92:LEU:HD23 | 20:AT:92:LEU:HA     | 1.67                     | 0.41              |
| 25:AY:8:U:H5'     | 25:AY:48:C:OP2      | 2.21                     | 0.41              |
| 28:BB:11:C:P      | 49:B0:72:ARG:HD2    | 2.61                     | 0.41              |
| 54:B5:33:CYS:SG   | 54:B5:33:CYS:O      | 2.78                     | 0.41              |
| 55:B6:11:LEU:HD12 | 55:B6:12:GLU:N      | 2.35                     | 0.41              |
| 27:BA:115:C:C4    | 27:BA:116:C:H5      | 2.39                     | 0.41              |
| 27:BA:1283:G:N2   | 27:BA:1286:A:C8     | 2.88                     | 0.41              |
| 27:BA:1407:C:O2   | 27:BA:1407:C:H2'    | 2.20                     | 0.41              |
| 27:BA:1450:G:C2'  | 27:BA:1450(A):C:O5' | 2.68                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:1465:G:H4'  | 27:BA:1528:A:H1'   | 2.02                     | 0.41              |
| 27:BA:1465:G:C5'  | 27:BA:1528:A:H1'   | 2.51                     | 0.41              |
| 27:BA:1613:G:C6   | 27:BA:1619:G:C6    | 3.09                     | 0.41              |
| 27:BA:1665:A:N6   | 27:BA:1666:G:C6    | 2.88                     | 0.41              |
| 27:BA:1905:C:N4   | 27:BA:1930:G:C2    | 2.88                     | 0.41              |
| 27:BA:193:U:C2'   | 27:BA:194:G:H5'    | 2.51                     | 0.41              |
| 27:BA:1765:C:N4   | 27:BA:1987:G:H1    | 2.19                     | 0.41              |
| 27:BA:1992:G:C4   | 27:BA:1997:G:C6    | 3.09                     | 0.41              |
| 27:BA:1658:C:N4   | 27:BA:2002:G:H1    | 2.19                     | 0.41              |
| 27:BA:2007:C:O2   | 27:BA:2007:C:H2'   | 2.21                     | 0.41              |
| 27:BA:2029:G:O6   | 27:BA:2032:G:H3'   | 2.20                     | 0.41              |
| 27:BA:2476:A:N1   | 27:BA:2477:C:C5    | 2.89                     | 0.41              |
| 27:BA:2848:G:O2'  | 27:BA:2849:U:H5'   | 2.21                     | 0.41              |
| 27:BA:2720:U:C4   | 27:BA:2873:A:N7    | 2.89                     | 0.41              |
| 27:BA:557:U:O2'   | 27:BA:558:G:C5'    | 2.68                     | 0.41              |
| 27:BA:627:A:H8    | 27:BA:627:A:OP1    | 2.04                     | 0.41              |
| 27:BA:732:C:O2'   | 27:BA:733:G:H5'    | 2.20                     | 0.41              |
| 27:BA:766:C:H2'   | 27:BA:767:U:H6     | 1.86                     | 0.41              |
| 28:BB:70:C:H42    | 28:BB:107:G:H1     | 1.69                     | 0.41              |
| 29:BC:169:GLY:O   | 29:BC:170:ALA:C    | 2.59                     | 0.41              |
| 30:BD:33:LEU:HD12 | 30:BD:33:LEU:N     | 2.25                     | 0.41              |
| 31:BE:128:SER:OG  | 31:BE:129:HIS:ND1  | 2.45                     | 0.41              |
| 31:BE:200:GLU:HG2 | 31:BE:201:THR:H    | 1.85                     | 0.41              |
| 31:BE:34:VAL:CG2  | 31:BE:34:VAL:O     | 2.69                     | 0.41              |
| 32:BF:111:ALA:HB2 | 32:BF:206:ILE:HG21 | 2.02                     | 0.41              |
| 32:BF:53:THR:HG22 | 32:BF:55:GLY:N     | 2.34                     | 0.41              |
| 33:BG:105:LYS:C   | 33:BG:107:LEU:N    | 2.74                     | 0.41              |
| 33:BG:51:ARG:CA   | 33:BG:51:ARG:HE    | 2.34                     | 0.41              |
| 34:BH:127:GLU:OE2 | 34:BH:130:ARG:NH2  | 2.54                     | 0.41              |
| 34:BH:137:ASP:O   | 34:BH:138:LYS:HB2  | 2.20                     | 0.41              |
| 34:BH:80:SER:O    | 34:BH:81:GLU:CB    | 2.68                     | 0.41              |
| 35:BI:29:TYR:O    | 35:BI:33:ARG:HD2   | 2.21                     | 0.41              |
| 35:BI:68:LEU:HA   | 35:BI:71:ILE:HD11  | 2.03                     | 0.41              |
| 35:BI:88:ILE:O    | 35:BI:89:TYR:CD2   | 2.74                     | 0.41              |
| 37:BO:97:ARG:CA   | 37:BO:117:LEU:HD22 | 2.51                     | 0.41              |
| 40:BR:22:ARG:C    | 40:BR:24:GLN:N     | 2.74                     | 0.41              |
| 40:BR:45:ARG:O    | 40:BR:47:PHE:N     | 2.54                     | 0.41              |
| 43:BU:76:TYR:O    | 43:BU:77:SER:C     | 2.58                     | 0.41              |
| 43:BU:95:LEU:HD13 | 44:BV:4:ILE:CG2    | 2.51                     | 0.41              |
| 44:BV:18:LEU:CG   | 44:BV:19:LYS:H     | 2.33                     | 0.41              |
| 47:BY:98:VAL:HG12 | 47:BY:98:VAL:O     | 2.20                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:BZ:44:ASP:C    | 48:BZ:46:VAL:N     | 2.73                     | 0.41              |
| 48:BZ:69:LEU:HD23 | 48:BZ:69:LEU:HA    | 1.88                     | 0.41              |
| 1:CA:1061:G:C6    | 1:CA:1197:G:C6     | 3.09                     | 0.41              |
| 1:CA:119:A:N7     | 1:CA:288:A:C2      | 2.89                     | 0.41              |
| 1:CA:1353:G:O2'   | 1:CA:1354:C:H5'    | 2.20                     | 0.41              |
| 1:CA:1473:A:H2'   | 1:CA:1474:G:C8     | 2.55                     | 0.41              |
| 1:CA:1498:U:H5''  | 1:CA:1499:A:OP1    | 2.20                     | 0.41              |
| 1:CA:288:A:H2'    | 1:CA:289:G:H4'     | 2.03                     | 0.41              |
| 1:CA:342:C:H2'    | 1:CA:343:U:O4'     | 2.21                     | 0.41              |
| 1:CA:548:G:H5''   | 1:CA:548:G:H8      | 1.86                     | 0.41              |
| 1:CA:563:A:C8     | 1:CA:567:G:O4'     | 2.74                     | 0.41              |
| 1:CA:608:A:H2'    | 1:CA:609:A:O4'     | 2.20                     | 0.41              |
| 1:CA:607:A:O2'    | 1:CA:608:A:H5'     | 2.21                     | 0.41              |
| 1:CA:689:C:H4'    | 1:CA:705:U:H1'     | 2.02                     | 0.41              |
| 1:CA:707:C:O2'    | 1:CA:708:C:H5'     | 2.21                     | 0.41              |
| 1:CA:710:G:N1     | 1:CA:711:G:C5      | 2.89                     | 0.41              |
| 1:CA:71:C:C2'     | 1:CA:72:C:H5'      | 2.51                     | 0.41              |
| 1:CA:834:C:N4     | 1:CA:853:G:C6      | 2.89                     | 0.41              |
| 1:CA:913:A:O2'    | 1:CA:914:A:P       | 2.79                     | 0.41              |
| 1:CA:926:G:C6     | 1:CA:1505:G:C5     | 3.08                     | 0.41              |
| 2:CB:144:ARG:HG3  | 2:CB:145:LEU:N     | 2.36                     | 0.41              |
| 1:CA:1190:G:OP1   | 3:CC:4:LYS:HA      | 2.21                     | 0.41              |
| 5:CE:129:ILE:O    | 5:CE:132:ALA:HB3   | 2.21                     | 0.41              |
| 7:CG:75:VAL:HG11  | 7:CG:144:MET:HB3   | 2.02                     | 0.41              |
| 10:CJ:8:LEU:HD23  | 10:CJ:96:ILE:HA    | 2.02                     | 0.41              |
| 11:CK:27:ASN:CG   | 11:CK:28:THR:N     | 2.74                     | 0.41              |
| 11:CK:52:GLY:H    | 11:CK:55:LYS:NZ    | 2.19                     | 0.41              |
| 11:CK:57:THR:HG22 | 11:CK:60:ALA:H     | 1.85                     | 0.41              |
| 12:CL:114:ARG:CG  | 12:CL:114:ARG:HH11 | 2.33                     | 0.41              |
| 12:CL:99:ARG:HE   | 12:CL:99:ARG:HB3   | 1.54                     | 0.41              |
| 14:CN:57:ARG:CG   | 14:CN:58:LYS:N     | 2.82                     | 0.41              |
| 18:CR:55:ARG:HH11 | 18:CR:55:ARG:HG3   | 1.84                     | 0.41              |
| 19:CS:41:VAL:HA   | 19:CS:42:PRO:HD3   | 1.77                     | 0.41              |
| 19:CS:38:SER:O    | 19:CS:70:LYS:HA    | 2.20                     | 0.41              |
| 20:CT:50:GLU:N    | 20:CT:100:ILE:HG12 | 2.34                     | 0.41              |
| 20:CT:60:GLU:O    | 20:CT:64:ASP:HB2   | 2.21                     | 0.41              |
| 1:CA:188:C:O4'    | 20:CT:89:ARG:NH2   | 2.53                     | 0.41              |
| 23:CW:48:C:H42    | 23:CW:64:G:H1      | 1.68                     | 0.41              |
| 23:CW:66:A:C6     | 23:CW:67:C:N4      | 2.88                     | 0.41              |
| 24:CX:7:G:C6      | 24:CX:49:G:N7      | 2.89                     | 0.41              |
| 50:D1:7:ILE:HD13  | 50:D1:62:VAL:CB    | 2.49                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:D3:31:LEU:HA    | 52:D3:31:LEU:HD23  | 1.84                     | 0.41              |
| 53:D4:40:ILE:O     | 53:D4:41:ILE:HD13  | 2.20                     | 0.41              |
| 54:D5:37:LYS:O     | 54:D5:38:ALA:O     | 2.38                     | 0.41              |
| 57:D8:53:PRO:O     | 57:D8:55:ALA:N     | 2.53                     | 0.41              |
| 27:DA:1017:G:H2'   | 27:DA:1018:C:H5'   | 2.00                     | 0.41              |
| 27:DA:1197:G:O2'   | 27:DA:1198:U:C5'   | 2.64                     | 0.41              |
| 27:DA:1300:U:C4    | 27:DA:1626:G:N7    | 2.88                     | 0.41              |
| 27:DA:1301:A:H62   | 27:DA:1641:A:N6    | 2.18                     | 0.41              |
| 27:DA:1696:G:H2'   | 27:DA:1697:G:O4'   | 2.21                     | 0.41              |
| 27:DA:1897:G:H2'   | 27:DA:1898:U:O4'   | 2.21                     | 0.41              |
| 27:DA:2031:A:O2'   | 27:DA:2032:G:OP2   | 2.36                     | 0.41              |
| 27:DA:2241:A:O2'   | 27:DA:2242:G:H5'   | 2.20                     | 0.41              |
| 27:DA:2281:C:O2'   | 27:DA:2282:G:H5'   | 2.21                     | 0.41              |
| 27:DA:2476:A:N1    | 27:DA:2477:C:C5    | 2.89                     | 0.41              |
| 27:DA:250:G:H2'    | 27:DA:251:A:C8     | 2.56                     | 0.41              |
| 27:DA:271(T):C:H2' | 27:DA:271(U):G:O4' | 2.20                     | 0.41              |
| 27:DA:323:G:C6     | 27:DA:333:G:C5     | 3.09                     | 0.41              |
| 27:DA:418:G:H2'    | 27:DA:419:C:C6     | 2.56                     | 0.41              |
| 27:DA:524:U:O2'    | 27:DA:525:U:H5'    | 2.21                     | 0.41              |
| 27:DA:698:C:OP1    | 27:DA:1634:A:N6    | 2.40                     | 0.41              |
| 29:DC:100:ILE:CD1  | 29:DC:132:GLY:HA3  | 2.45                     | 0.41              |
| 30:DD:33:LEU:O     | 30:DD:34:VAL:CG1   | 2.66                     | 0.41              |
| 31:DE:37:ARG:HB2   | 31:DE:46:ALA:CA    | 2.50                     | 0.41              |
| 31:DE:9:VAL:O      | 31:DE:192:ASN:ND2  | 2.54                     | 0.41              |
| 32:DF:110:LEU:C    | 32:DF:110:LEU:CD1  | 2.90                     | 0.41              |
| 32:DF:156:LEU:HD12 | 32:DF:193:VAL:O    | 2.20                     | 0.41              |
| 32:DF:58:ALA:O     | 32:DF:59:TYR:O     | 2.39                     | 0.41              |
| 33:DG:105:LYS:HD2  | 33:DG:142:PRO:HG3  | 2.03                     | 0.41              |
| 28:DB:42:C:H4'     | 33:DG:67:LYS:O     | 2.20                     | 0.41              |
| 34:DH:113:VAL:HG12 | 34:DH:115:VAL:CG2  | 2.51                     | 0.41              |
| 34:DH:54:ARG:HA    | 34:DH:55:PRO:HD2   | 1.86                     | 0.41              |
| 37:DO:37:ASP:O     | 37:DO:61:VAL:HG23  | 2.21                     | 0.41              |
| 37:DO:91:LEU:HA    | 37:DO:91:LEU:HD13  | 1.88                     | 0.41              |
| 38:DP:23:PRO:CG    | 38:DP:33:ARG:NE    | 2.84                     | 0.41              |
| 38:DP:46:LYS:O     | 38:DP:47:ASP:HB2   | 2.20                     | 0.41              |
| 38:DP:58:THR:O     | 38:DP:61:ARG:CD    | 2.69                     | 0.41              |
| 39:DQ:27:VAL:HB    | 39:DQ:137:TYR:CD1  | 2.56                     | 0.41              |
| 41:DS:35:ILE:O     | 41:DS:53:SER:HB2   | 2.20                     | 0.41              |
| 42:DT:19:LEU:HD12  | 42:DT:19:LEU:N     | 2.33                     | 0.41              |
| 48:DZ:19:ARG:O     | 48:DZ:21:GLY:N     | 2.54                     | 0.41              |
| 48:DZ:44:ASP:CG    | 48:DZ:48:ARG:HG2   | 2.42                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1363(A):A:OP1 | 1:AA:1363(A):A:C8 | 2.74                     | 0.41              |
| 1:AA:137:C:H2'     | 1:AA:138:G:H5'    | 2.03                     | 0.41              |
| 1:AA:219:C:C4      | 1:AA:220:G:C8     | 3.10                     | 0.41              |
| 1:AA:366:C:O2'     | 1:AA:367:U:H5''   | 2.21                     | 0.41              |
| 1:AA:374:A:H2'     | 1:AA:375:U:H6     | 1.86                     | 0.41              |
| 1:AA:60:A:H8       | 1:AA:60:A:P       | 2.44                     | 0.41              |
| 1:AA:787:A:C5      | 1:AA:788:U:C5     | 3.09                     | 0.41              |
| 1:AA:813:U:OP2     | 1:AA:816:A:N6     | 2.54                     | 0.41              |
| 1:AA:973:G:C3'     | 1:AA:974:A:H5''   | 2.47                     | 0.41              |
| 1:AA:977:A:H1'     | 1:AA:982:U:O4     | 2.21                     | 0.41              |
| 2:AB:80:ILE:HD13   | 2:AB:211:ILE:CG2  | 2.51                     | 0.41              |
| 3:AC:54:ARG:HH11   | 3:AC:54:ARG:HG2   | 1.86                     | 0.41              |
| 1:AA:15:G:C4'      | 5:AE:24:ARG:HH12  | 2.17                     | 0.41              |
| 8:AH:14:ARG:HG3    | 8:AH:18:ARG:NH1   | 2.36                     | 0.41              |
| 9:AI:99:LEU:HB3    | 9:AI:101:PHE:HE1  | 1.80                     | 0.41              |
| 11:AK:33:THR:C     | 11:AK:40:ILE:HD11 | 2.42                     | 0.41              |
| 12:AL:124:GLU:O    | 12:AL:125:ALA:C   | 2.59                     | 0.41              |
| 12:AL:24:LEU:N     | 12:AL:24:LEU:HD13 | 2.35                     | 0.41              |
| 12:AL:57:LEU:N     | 12:AL:57:LEU:HD22 | 2.36                     | 0.41              |
| 16:AP:23:ASP:OD1   | 16:AP:23:ASP:C    | 2.59                     | 0.41              |
| 18:AR:52:PRO:O     | 18:AR:56:THR:HG23 | 2.21                     | 0.41              |
| 50:B1:53:VAL:CG2   | 50:B1:74:VAL:HG22 | 2.51                     | 0.41              |
| 51:B2:13:ALA:HA    | 51:B2:16:LEU:CD1  | 2.51                     | 0.41              |
| 55:B6:30:THR:O     | 55:B6:31:PRO:C    | 2.59                     | 0.41              |
| 27:BA:592:G:O2'    | 57:B8:4:MET:HB2   | 2.21                     | 0.41              |
| 58:B9:29:ASN:OD1   | 58:B9:31:LYS:HB3  | 2.21                     | 0.41              |
| 27:BA:1200:C:C2    | 27:BA:1246:A:C2   | 3.08                     | 0.41              |
| 27:BA:1740:G:O2'   | 27:BA:1741:A:H5'  | 2.21                     | 0.41              |
| 27:BA:173:G:C2     | 27:BA:174:C:C2    | 3.09                     | 0.41              |
| 27:BA:781:A:C2     | 27:BA:1776:G:N3   | 2.89                     | 0.41              |
| 27:BA:1798:U:O2    | 27:BA:1802:A:H2   | 2.03                     | 0.41              |
| 27:BA:1836:C:C2'   | 27:BA:1837:C:H5'  | 2.51                     | 0.41              |
| 27:BA:2265:U:O2    | 27:BA:2276:G:C2   | 2.74                     | 0.41              |
| 27:BA:2544:G:H2'   | 27:BA:2545:G:H8   | 1.86                     | 0.41              |
| 27:BA:2792:G:C8    | 27:BA:2893:G:O6   | 2.74                     | 0.41              |
| 27:BA:301:G:O6     | 27:BA:316:C:N4    | 2.55                     | 0.41              |
| 27:BA:491:G:H2'    | 27:BA:492:A:O5'   | 2.20                     | 0.41              |
| 27:BA:60:G:C8      | 27:BA:63:U:C5     | 3.09                     | 0.41              |
| 27:BA:675:A:N6     | 27:BA:676:A:N6    | 2.69                     | 0.41              |
| 27:BA:681:G:H2'    | 27:BA:682:G:O4'   | 2.21                     | 0.41              |
| 27:BA:88:G:N2      | 27:BA:89:G:C4     | 2.89                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BA:942:G:H2'    | 27:BA:943:U:C5'   | 2.50                     | 0.41              |
| 28:BB:25:A:N3      | 28:BB:25:A:H2'    | 2.35                     | 0.41              |
| 29:BC:83:ILE:HA    | 29:BC:94:VAL:CG2  | 2.47                     | 0.41              |
| 30:BD:142:VAL:HG23 | 30:BD:143:HIS:N   | 2.36                     | 0.41              |
| 30:BD:211:ARG:HA   | 30:BD:214:TRP:CD2 | 2.56                     | 0.41              |
| 30:BD:84:TYR:CD2   | 30:BD:85:ASP:N    | 2.89                     | 0.41              |
| 32:BF:61:GLY:O     | 32:BF:62:ARG:O    | 2.38                     | 0.41              |
| 32:BF:51:THR:HB    | 32:BF:88:VAL:HG11 | 2.03                     | 0.41              |
| 33:BG:154:GLY:C    | 33:BG:155:MET:HG2 | 2.41                     | 0.41              |
| 33:BG:176:LEU:HD12 | 33:BG:176:LEU:H   | 1.86                     | 0.41              |
| 35:BI:48:GLU:O     | 35:BI:52:ARG:HG2  | 2.21                     | 0.41              |
| 35:BI:91:SER:O     | 35:BI:92:VAL:CG1  | 2.68                     | 0.41              |
| 35:BI:95:LYS:O     | 35:BI:98:ALA:HB3  | 2.21                     | 0.41              |
| 27:BA:662:G:P      | 38:BP:18:ARG:HD2  | 2.61                     | 0.41              |
| 38:BP:21:ARG:O     | 38:BP:23:PRO:HD3  | 2.20                     | 0.41              |
| 38:BP:6:LEU:N      | 38:BP:6:LEU:HD23  | 2.31                     | 0.41              |
| 39:BQ:26:TYR:O     | 39:BQ:26:TYR:CD1  | 2.74                     | 0.41              |
| 42:BT:109:GLU:HA   | 42:BT:112:ARG:CD  | 2.50                     | 0.41              |
| 42:BT:81:PRO:HD2   | 42:BT:82:LEU:CD1  | 2.51                     | 0.41              |
| 47:BY:8:LYS:N      | 47:BY:8:LYS:CD    | 2.82                     | 0.41              |
| 1:CA:1009:G:C6     | 1:CA:1021:G:C5    | 3.09                     | 0.41              |
| 1:CA:1311:G:C2     | 1:CA:1327:C:N3    | 2.89                     | 0.41              |
| 1:CA:189(B):C:H2'  | 1:CA:189(C):C:C6  | 2.55                     | 0.41              |
| 1:CA:201:C:N4      | 1:CA:203:U:N3     | 2.69                     | 0.41              |
| 1:CA:271:C:H2'     | 1:CA:272:C:C6     | 2.56                     | 0.41              |
| 1:CA:344:A:C3'     | 1:CA:346:G:O6     | 2.69                     | 0.41              |
| 1:CA:619:U:O4      | 4:CD:135:LEU:HD11 | 2.21                     | 0.41              |
| 1:CA:690:G:H2'     | 1:CA:691:G:N9     | 2.36                     | 0.41              |
| 1:CA:709:G:H2'     | 1:CA:710:G:C8     | 2.56                     | 0.41              |
| 1:CA:722:A:O2'     | 1:CA:723:U:H2'    | 2.21                     | 0.41              |
| 1:CA:752:G:O2'     | 1:CA:753:A:H5'    | 2.21                     | 0.41              |
| 1:CA:832:C:H2'     | 1:CA:833:U:O4'    | 2.21                     | 0.41              |
| 1:CA:892:A:C2      | 1:CA:893:C:C2     | 3.09                     | 0.41              |
| 2:CB:167:PRO:CD    | 2:CB:188:ALA:HB2  | 2.51                     | 0.41              |
| 5:CE:20:GLN:O      | 5:CE:23:GLY:O     | 2.39                     | 0.41              |
| 6:CF:27:GLN:O      | 6:CF:28:ARG:C     | 2.59                     | 0.41              |
| 8:CH:97:VAL:HA     | 8:CH:100:ILE:CD1  | 2.51                     | 0.41              |
| 9:CI:63:ILE:HD13   | 9:CI:77:ILE:HG23  | 2.02                     | 0.41              |
| 12:CL:53:ALA:O     | 12:CL:64:THR:HA   | 2.21                     | 0.41              |
| 13:CM:8:GLU:OE2    | 13:CM:22:ILE:HG23 | 2.21                     | 0.41              |
| 16:CP:68:ASP:HA    | 16:CP:71:ARG:HD3  | 2.03                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:CR:65:ILE:H     | 18:CR:65:ILE:HG13 | 1.74                     | 0.41              |
| 24:CX:24:U:O2'     | 27:DA:1923:U:H5'' | 2.20                     | 0.41              |
| 49:D0:53:MET:CE    | 49:D0:57:PHE:HD1  | 2.33                     | 0.41              |
| 55:D6:17:LYS:CB    | 55:D6:18:ARG:NH1  | 2.81                     | 0.41              |
| 27:DA:1037:G:H2'   | 27:DA:1038:C:O4'  | 2.21                     | 0.41              |
| 27:DA:1167:U:H1'   | 27:DA:1183:G:N2   | 2.34                     | 0.41              |
| 27:DA:1191:G:H21   | 27:DA:1192:G:H1'  | 1.86                     | 0.41              |
| 27:DA:1209:G:O2'   | 27:DA:1237:A:N6   | 2.40                     | 0.41              |
| 27:DA:1458:C:C4'   | 27:DA:1459:G:O5'  | 2.67                     | 0.41              |
| 27:DA:1526:G:C6    | 27:DA:1527:G:C2   | 3.09                     | 0.41              |
| 27:DA:1941:C:C2    | 27:DA:1965:C:C2   | 3.08                     | 0.41              |
| 27:DA:1954:G:H1'   | 27:DA:1956:U:O4   | 2.21                     | 0.41              |
| 27:DA:1678:G:H21   | 27:DA:1989:G:H1   | 1.67                     | 0.41              |
| 27:DA:2070:G:C6    | 27:DA:2442:C:C4   | 3.09                     | 0.41              |
| 27:DA:2249:U:O2'   | 27:DA:2250:G:OP1  | 2.33                     | 0.41              |
| 27:DA:242:G:C8     | 57:D8:5:LYS:HG2   | 2.56                     | 0.41              |
| 27:DA:2555:U:O4    | 27:DA:2556:C:O2   | 2.38                     | 0.41              |
| 27:DA:2566:A:O2'   | 27:DA:2567:G:OP2  | 2.31                     | 0.41              |
| 27:DA:2673:G:H2'   | 27:DA:2674:G:H8   | 1.85                     | 0.41              |
| 27:DA:271(D):G:H2' | 27:DA:271(E):U:H6 | 1.85                     | 0.41              |
| 27:DA:2682:U:O4    | 27:DA:2728:U:H1'  | 2.21                     | 0.41              |
| 27:DA:2747:G:H21   | 27:DA:2748:A:N6   | 2.18                     | 0.41              |
| 27:DA:2770:G:C5'   | 27:DA:2771:C:OP2  | 2.69                     | 0.41              |
| 27:DA:2855:C:H2'   | 27:DA:2856:C:C6   | 2.53                     | 0.41              |
| 27:DA:2801:A:O2'   | 27:DA:2895:U:H4'  | 2.21                     | 0.41              |
| 27:DA:385:C:O2     | 27:DA:390:A:C2    | 2.74                     | 0.41              |
| 27:DA:463:G:N2     | 27:DA:467:G:C4    | 2.89                     | 0.41              |
| 27:DA:489:G:N3     | 27:DA:1284:A:C6   | 2.89                     | 0.41              |
| 27:DA:513:A:C2     | 27:DA:514:A:N9    | 2.89                     | 0.41              |
| 27:DA:530:G:C2     | 27:DA:2021:C:O2'  | 2.68                     | 0.41              |
| 27:DA:620:G:H5'    | 27:DA:621:A:OP1   | 2.21                     | 0.41              |
| 27:DA:686:G:C8     | 56:D7:7:PRO:HA    | 2.55                     | 0.41              |
| 27:DA:695:G:C4     | 27:DA:768:G:N1    | 2.89                     | 0.41              |
| 27:DA:775:G:N1     | 27:DA:787:U:C4    | 2.89                     | 0.41              |
| 27:DA:994:C:OP1    | 43:DU:53:ARG:NH2  | 2.54                     | 0.41              |
| 29:DC:39:GLU:HA    | 29:DC:179:SER:O   | 2.21                     | 0.41              |
| 30:DD:138:VAL:HG12 | 30:DD:168:ARG:NE  | 2.35                     | 0.41              |
| 31:DE:59:VAL:HG21  | 31:DE:63:LEU:CD1  | 2.51                     | 0.41              |
| 32:DF:9:ILE:CG1    | 32:DF:14:PRO:HA   | 2.49                     | 0.41              |
| 33:DG:115:ARG:HH12 | 33:DG:136:ARG:HD3 | 1.86                     | 0.41              |
| 33:DG:31:VAL:CG2   | 33:DG:32:PRO:HD2  | 2.50                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DH:44:VAL:C     | 34:DH:46:GLU:H     | 2.25                     | 0.41              |
| 34:DH:70:THR:HB    | 34:DH:71:LEU:H     | 1.57                     | 0.41              |
| 35:DI:39:ALA:O     | 35:DI:40:THR:C     | 2.59                     | 0.41              |
| 37:DO:79:PHE:N     | 37:DO:79:PHE:CD1   | 2.89                     | 0.41              |
| 38:DP:106:LEU:HD12 | 38:DP:106:LEU:HA   | 1.96                     | 0.41              |
| 40:DR:63:ARG:NH1   | 40:DR:63:ARG:HG3   | 2.36                     | 0.41              |
| 40:DR:26:LYS:HG2   | 40:DR:70:LEU:HD23  | 2.02                     | 0.41              |
| 42:DT:74:ARG:O     | 42:DT:75:ILE:HG13  | 2.21                     | 0.41              |
| 47:DY:45:VAL:CG1   | 47:DY:46:LYS:N     | 2.84                     | 0.41              |
| 47:DY:87:LYS:HG3   | 47:DY:88:LYS:N     | 2.36                     | 0.41              |
| 39:DQ:108:GLY:CA   | 48:DZ:115:VAL:HG11 | 2.47                     | 0.41              |
| 48:DZ:94:PRO:O     | 48:DZ:95:VAL:O     | 2.39                     | 0.41              |
| 1:AA:1049:U:HO2'   | 1:AA:1050:G:P      | 2.44                     | 0.40              |
| 1:AA:1058:G:C5     | 1:AA:1059:C:C4     | 3.09                     | 0.40              |
| 1:AA:1104:G:H4'    | 2:AB:111:ARG:HH11  | 1.85                     | 0.40              |
| 1:AA:1049:U:O2     | 1:AA:1201:A:C4     | 2.74                     | 0.40              |
| 1:AA:1243:C:H2'    | 1:AA:1244:C:C6     | 2.51                     | 0.40              |
| 1:AA:1346:A:C8     | 1:AA:1348:U:C2     | 3.09                     | 0.40              |
| 1:AA:1351:U:H2'    | 1:AA:1352:C:C6     | 2.56                     | 0.40              |
| 1:AA:1458:G:C2'    | 1:AA:1459:C:H5'    | 2.51                     | 0.40              |
| 1:AA:177:C:OP1     | 20:AT:65:LYS:NZ    | 2.51                     | 0.40              |
| 1:AA:129(A):G:H22  | 1:AA:189(E):U:H1'  | 1.85                     | 0.40              |
| 1:AA:138:G:N2      | 1:AA:226:G:C4      | 2.89                     | 0.40              |
| 1:AA:323:U:O2      | 1:AA:323:U:H2'     | 2.21                     | 0.40              |
| 1:AA:414:A:H2'     | 1:AA:415:A:O4'     | 2.21                     | 0.40              |
| 1:AA:528:C:O2'     | 1:AA:529:G:H5'     | 2.21                     | 0.40              |
| 1:AA:541:G:O2'     | 1:AA:542:G:H5'     | 2.20                     | 0.40              |
| 1:AA:545:C:O2'     | 1:AA:549:C:OP1     | 2.38                     | 0.40              |
| 1:AA:841:U:H2'     | 1:AA:848:C:O4'     | 2.21                     | 0.40              |
| 2:AB:178:ARG:CG    | 2:AB:178:ARG:HH11  | 2.32                     | 0.40              |
| 2:AB:167:PRO:HG3   | 2:AB:188:ALA:HB2   | 2.04                     | 0.40              |
| 2:AB:80:ILE:HD12   | 2:AB:212:GLN:HA    | 2.02                     | 0.40              |
| 3:AC:24:ALA:CB     | 3:AC:32:LEU:HD12   | 2.51                     | 0.40              |
| 1:AA:619:U:O4      | 4:AD:135:LEU:HD11  | 2.20                     | 0.40              |
| 4:AD:162:LEU:HA    | 4:AD:165:MET:HG2   | 2.02                     | 0.40              |
| 4:AD:196:LEU:O     | 4:AD:198:VAL:N     | 2.53                     | 0.40              |
| 7:AG:108:ALA:C     | 7:AG:110:GLN:H     | 2.25                     | 0.40              |
| 7:AG:151:TYR:HA    | 7:AG:153:HIS:HE1   | 1.80                     | 0.40              |
| 8:AH:12:ARG:NH1    | 8:AH:26:VAL:HA     | 2.36                     | 0.40              |
| 8:AH:72:PRO:O      | 8:AH:73:ASP:C      | 2.60                     | 0.40              |
| 9:AI:116:LYS:O     | 9:AI:118:LYS:N     | 2.54                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AK:79:SER:HB2   | 11:AK:106:LYS:CD   | 2.51                     | 0.40              |
| 3:AC:30:ARG:CZ     | 14:AN:35:ARG:O     | 2.69                     | 0.40              |
| 14:AN:51:GLY:C     | 14:AN:53:LEU:N     | 2.71                     | 0.40              |
| 15:AO:51:HIS:ND1   | 15:AO:51:HIS:N     | 2.69                     | 0.40              |
| 20:AT:104:LEU:HD23 | 20:AT:105:SER:N    | 2.36                     | 0.40              |
| 24:AX:49:G:H1      | 24:AX:65:C:H42     | 1.67                     | 0.40              |
| 25:AY:4:G:N2       | 25:AY:69:C:C2      | 2.89                     | 0.40              |
| 51:B2:24:LEU:HD11  | 51:B2:28:LYS:CE    | 2.51                     | 0.40              |
| 51:B2:32:LEU:O     | 51:B2:35:LEU:CB    | 2.68                     | 0.40              |
| 52:B3:29:ARG:H     | 52:B3:33:GLN:NE2   | 2.18                     | 0.40              |
| 52:B3:22:ALA:CB    | 52:B3:46:ASN:HD22  | 2.34                     | 0.40              |
| 27:BA:2611:U:O2    | 54:B5:3:LYS:HE3    | 2.20                     | 0.40              |
| 55:B6:11:LEU:HD12  | 55:B6:12:GLU:O     | 2.21                     | 0.40              |
| 55:B6:15:GLU:OE2   | 55:B6:18:ARG:CD    | 2.69                     | 0.40              |
| 27:BA:1049:C:N4    | 27:BA:1111:A:N1    | 2.69                     | 0.40              |
| 27:BA:14:A:H2'     | 27:BA:15:G:O4'     | 2.21                     | 0.40              |
| 27:BA:1448:G:N3    | 27:BA:1528(A):A:H2 | 2.19                     | 0.40              |
| 27:BA:177:G:O2'    | 27:BA:178:G:OP1    | 2.36                     | 0.40              |
| 26:AZ:3:SER:HB2    | 27:BA:1913:A:O2'   | 2.19                     | 0.40              |
| 27:BA:2064:C:H2'   | 27:BA:2065:C:C6    | 2.56                     | 0.40              |
| 27:BA:2259:G:N2    | 27:BA:2282:G:C6    | 2.89                     | 0.40              |
| 27:BA:2545:G:N3    | 27:BA:2565:A:H2    | 2.18                     | 0.40              |
| 27:BA:2706:G:O2'   | 40:BR:64:ARG:HD3   | 2.20                     | 0.40              |
| 27:BA:281:G:N2     | 27:BA:358:U:C5     | 2.90                     | 0.40              |
| 27:BA:610:G:O2'    | 27:BA:611:C:H5'    | 2.21                     | 0.40              |
| 27:BA:68:G:C6      | 27:BA:69:C:C4      | 3.08                     | 0.40              |
| 27:BA:819:A:OP2    | 27:BA:1187:G:N2    | 2.38                     | 0.40              |
| 28:BB:16:G:N3      | 28:BB:17:C:C6      | 2.89                     | 0.40              |
| 28:BB:83:G:H4'     | 52:B3:52:HIS:HD2   | 1.83                     | 0.40              |
| 30:BD:185:VAL:HG12 | 30:BD:186:HIS:N    | 2.36                     | 0.40              |
| 31:BE:77:ILE:CG2   | 31:BE:78:LEU:HD23  | 2.51                     | 0.40              |
| 32:BF:13:SER:HA    | 32:BF:14:PRO:HD3   | 1.73                     | 0.40              |
| 32:BF:160:ASN:ND2  | 32:BF:162:LEU:N    | 2.65                     | 0.40              |
| 35:BI:42:SER:C     | 35:BI:44:LEU:N     | 2.74                     | 0.40              |
| 39:BQ:68:ILE:HD13  | 39:BQ:103:MET:CE   | 2.51                     | 0.40              |
| 39:BQ:3:MET:O      | 39:BQ:5:ARG:N      | 2.54                     | 0.40              |
| 40:BR:118:GLU:HG3  | 40:BR:118:GLU:OXT  | 2.19                     | 0.40              |
| 42:BT:85:LYS:CB    | 42:BT:85:LYS:NZ    | 2.82                     | 0.40              |
| 1:CA:1136:U:H5''   | 1:CA:1137:C:C5     | 2.56                     | 0.40              |
| 1:CA:134:A:H61     | 16:CP:25:ARG:NH1   | 2.14                     | 0.40              |
| 1:CA:1439:C:H2'    | 1:CA:1440:C:O4'    | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:144:G:C2     | 1:CA:179:A:C2     | 3.10                     | 0.40              |
| 1:CA:187:C:O4'    | 20:CT:85:MET:HG3  | 2.21                     | 0.40              |
| 1:CA:243:A:H4'    | 1:CA:244:U:O5'    | 2.22                     | 0.40              |
| 1:CA:310:G:OP2    | 16:CP:27:LYS:NZ   | 2.50                     | 0.40              |
| 1:CA:334:C:O5'    | 1:CA:334:C:H6     | 2.04                     | 0.40              |
| 1:CA:507:C:P      | 1:CA:508:C:H3'    | 2.62                     | 0.40              |
| 1:CA:716:A:H2'    | 1:CA:717:C:O4'    | 2.21                     | 0.40              |
| 1:CA:719:C:H6     | 1:CA:720:C:C5     | 2.39                     | 0.40              |
| 1:CA:664:G:N2     | 1:CA:741:G:H1     | 2.04                     | 0.40              |
| 1:CA:832:C:HO2'   | 1:CA:833:U:H5'    | 1.84                     | 0.40              |
| 1:CA:244:U:C6     | 1:CA:894:G:C2     | 3.09                     | 0.40              |
| 1:CA:991:U:O2     | 1:CA:991:U:C2'    | 2.61                     | 0.40              |
| 2:CB:129:GLU:O    | 2:CB:130:ARG:HB2  | 2.21                     | 0.40              |
| 3:CC:159:GLY:HA3  | 3:CC:193:TYR:CE2  | 2.55                     | 0.40              |
| 4:CD:127:THR:HG22 | 4:CD:132:ARG:CB   | 2.51                     | 0.40              |
| 4:CD:154:ASN:N    | 4:CD:154:ASN:OD1  | 2.54                     | 0.40              |
| 4:CD:152:SER:O    | 4:CD:158:ILE:HG13 | 2.21                     | 0.40              |
| 5:CE:144:THR:O    | 5:CE:147:ASP:OD2  | 2.39                     | 0.40              |
| 6:CF:69:GLU:HG2   | 6:CF:70:ASP:N     | 2.36                     | 0.40              |
| 6:CF:4:TYR:CD1    | 6:CF:92:LYS:HA    | 2.55                     | 0.40              |
| 7:CG:137:LYS:O    | 7:CG:141:VAL:CG2  | 2.65                     | 0.40              |
| 7:CG:29:LYS:O     | 7:CG:105:VAL:HG21 | 2.21                     | 0.40              |
| 11:CK:57:THR:HB   | 11:CK:60:ALA:CB   | 2.51                     | 0.40              |
| 12:CL:27:ALA:HA   | 12:CL:28:PRO:HD3  | 1.89                     | 0.40              |
| 12:CL:55:VAL:O    | 12:CL:57:LEU:HD22 | 2.21                     | 0.40              |
| 13:CM:35:GLU:CG   | 13:CM:36:LYS:N    | 2.84                     | 0.40              |
| 20:CT:14:LYS:HA   | 20:CT:17:ARG:HE   | 1.85                     | 0.40              |
| 24:CX:17:C:C2'    | 24:CX:17(B):U:H5' | 2.51                     | 0.40              |
| 50:D1:51:VAL:HG13 | 50:D1:53:VAL:HG23 | 2.02                     | 0.40              |
| 55:D6:15:GLU:CD   | 55:D6:18:ARG:HG3  | 2.42                     | 0.40              |
| 55:D6:20:ASN:CG   | 55:D6:21:TYR:H    | 2.24                     | 0.40              |
| 27:DA:1024:G:OP2  | 27:DA:1026:U:OP1  | 2.39                     | 0.40              |
| 27:DA:1228:G:O2'  | 27:DA:1229:G:H5'  | 2.22                     | 0.40              |
| 27:DA:1309:G:H2'  | 27:DA:1310:G:H5'  | 2.02                     | 0.40              |
| 27:DA:1416:G:O2'  | 27:DA:1417:C:O4'  | 2.38                     | 0.40              |
| 27:DA:1459:G:H2'  | 27:DA:1459:G:N3   | 2.36                     | 0.40              |
| 27:DA:154(A):C:N4 | 27:DA:172:C:N4    | 2.53                     | 0.40              |
| 27:DA:1889:A:C2   | 27:DA:1890:A:C4   | 3.08                     | 0.40              |
| 27:DA:1905:C:H4'  | 27:DA:1928:A:C2   | 2.56                     | 0.40              |
| 27:DA:2069:G:N2   | 27:DA:2070:G:N9   | 2.69                     | 0.40              |
| 27:DA:2232:U:HO2' | 27:DA:2233:U:H5'  | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DA:2241:A:C6    | 27:DA:2242:G:C6    | 3.09                     | 0.40              |
| 27:DA:2360:A:C2    | 27:DA:2361:A:H1'   | 2.56                     | 0.40              |
| 25:CY:75:A:O2'     | 27:DA:2395:C:C2    | 2.73                     | 0.40              |
| 27:DA:2548:G:H2'   | 27:DA:2549:G:O5'   | 2.21                     | 0.40              |
| 27:DA:2552:U:O2    | 27:DA:2554:U:H5''  | 2.20                     | 0.40              |
| 27:DA:2588:G:H2'   | 27:DA:2589:A:C8    | 2.56                     | 0.40              |
| 27:DA:2595:G:N2    | 27:DA:2599:G:C5    | 2.89                     | 0.40              |
| 27:DA:382:G:C2     | 27:DA:393:C:C2     | 3.09                     | 0.40              |
| 27:DA:389:G:N1     | 38:DP:71:VAL:CG1   | 2.76                     | 0.40              |
| 27:DA:453:C:O2'    | 27:DA:472:A:N6     | 2.55                     | 0.40              |
| 27:DA:775:G:C2     | 27:DA:777:A:N6     | 2.89                     | 0.40              |
| 27:DA:7:G:H5''     | 36:DN:121:LYS:HZ1  | 1.86                     | 0.40              |
| 27:DA:942:G:N1     | 27:DA:943:U:C2     | 2.89                     | 0.40              |
| 27:DA:955:C:C2'    | 27:DA:956:G:H5'    | 2.50                     | 0.40              |
| 28:DB:114:C:H2'    | 28:DB:115:G:C8     | 2.56                     | 0.40              |
| 29:DC:54:SER:HB2   | 29:DC:55:ASP:H     | 1.74                     | 0.40              |
| 29:DC:72:VAL:HG21  | 29:DC:161:ILE:CA   | 2.50                     | 0.40              |
| 27:DA:1789:A:OP1   | 30:DD:222:ARG:HG3  | 2.21                     | 0.40              |
| 30:DD:24:ILE:O     | 30:DD:26:LYS:HD3   | 2.21                     | 0.40              |
| 31:DE:141:ILE:O    | 31:DE:150:VAL:HG22 | 2.20                     | 0.40              |
| 33:DG:11:TYR:HD2   | 33:DG:12:TYR:CD2   | 2.39                     | 0.40              |
| 35:DI:120:ILE:HG22 | 35:DI:121:LYS:N    | 2.36                     | 0.40              |
| 36:DN:126:PRO:HB2  | 36:DN:127:ASP:H    | 1.76                     | 0.40              |
| 36:DN:4:TYR:HB2    | 43:DU:64:ARG:CZ    | 2.51                     | 0.40              |
| 37:DO:11:ALA:CB    | 37:DO:64:ARG:NH2   | 2.84                     | 0.40              |
| 38:DP:95:VAL:HB    | 38:DP:100:LEU:HD21 | 2.03                     | 0.40              |
| 42:DT:2:ASN:O      | 42:DT:3:ARG:HG2    | 2.21                     | 0.40              |
| 42:DT:77:PRO:O     | 42:DT:78:LEU:HB3   | 2.21                     | 0.40              |
| 46:DX:43:VAL:O     | 46:DX:44:GLU:O     | 2.38                     | 0.40              |
| 1:AA:1002:G:H3'    | 1:AA:1003:G:C8     | 2.56                     | 0.40              |
| 1:AA:1117:G:H2'    | 1:AA:1118:C:H5'    | 2.04                     | 0.40              |
| 1:AA:1258:G:C4     | 1:AA:1259:C:C5     | 3.10                     | 0.40              |
| 1:AA:1279:A:C4'    | 1:AA:1280:A:OP1    | 2.69                     | 0.40              |
| 1:AA:1332:A:O2'    | 1:AA:1333:A:H5'    | 2.22                     | 0.40              |
| 1:AA:1420:C:H2'    | 1:AA:1421:G:C8     | 2.56                     | 0.40              |
| 1:AA:1494:G:C6     | 26:AZ:1:KBE:HAA    | 2.56                     | 0.40              |
| 1:AA:192:U:H2'     | 1:AA:193:C:H6      | 1.86                     | 0.40              |
| 1:AA:344:A:C3'     | 1:AA:346:G:O6      | 2.69                     | 0.40              |
| 1:AA:36:C:N4       | 1:AA:37:U:C4       | 2.89                     | 0.40              |
| 1:AA:454:C:H2'     | 1:AA:455:C:C5      | 2.55                     | 0.40              |
| 1:AA:533:A:H1'     | 1:AA:534:U:OP1     | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:577:G:H4'    | 1:AA:816:A:HO2'   | 1.85                     | 0.40              |
| 1:AA:62:U:C2      | 1:AA:63:C:C5      | 3.10                     | 0.40              |
| 1:AA:681:C:O2     | 1:AA:710:G:C2     | 2.73                     | 0.40              |
| 1:AA:796:C:OP1    | 11:AK:123:LYS:NZ  | 2.50                     | 0.40              |
| 1:AA:870:U:H4'    | 1:AA:871:U:O5'    | 2.21                     | 0.40              |
| 1:AA:966:G:O2'    | 1:AA:967:C:O5'    | 2.39                     | 0.40              |
| 2:AB:188:ALA:O    | 2:AB:202:PRO:HA   | 2.21                     | 0.40              |
| 2:AB:77:ALA:CB    | 2:AB:211:ILE:HD13 | 2.50                     | 0.40              |
| 3:AC:10:PHE:CD1   | 3:AC:10:PHE:O     | 2.74                     | 0.40              |
| 3:AC:173:VAL:N    | 3:AC:174:PRO:CD   | 2.85                     | 0.40              |
| 4:AD:162:LEU:HD12 | 4:AD:181:MET:CE   | 2.51                     | 0.40              |
| 5:AE:20:GLN:O     | 5:AE:21:ALA:O     | 2.39                     | 0.40              |
| 6:AF:8:ILE:HG23   | 6:AF:87:ARG:O     | 2.21                     | 0.40              |
| 1:AA:1378:C:H5''  | 7:AG:94:ARG:HH12  | 1.85                     | 0.40              |
| 10:AJ:22:LYS:C    | 10:AJ:22:LYS:CD   | 2.89                     | 0.40              |
| 1:AA:1061:G:H1'   | 10:AJ:56:HIS:CE1  | 2.57                     | 0.40              |
| 12:AL:27:ALA:CB   | 12:AL:30:ARG:NH2  | 2.84                     | 0.40              |
| 13:AM:48:LEU:HG   | 13:AM:53:VAL:HG23 | 2.03                     | 0.40              |
| 13:AM:76:ALA:CA   | 13:AM:79:LYS:NZ   | 2.84                     | 0.40              |
| 14:AN:32:SER:O    | 14:AN:40:CYS:HA   | 2.21                     | 0.40              |
| 16:AP:67:THR:H    | 16:AP:70:ALA:CB   | 2.34                     | 0.40              |
| 19:AS:64:GLU:O    | 19:AS:65:ASN:C    | 2.60                     | 0.40              |
| 20:AT:74:LYS:C    | 20:AT:76:ALA:N    | 2.73                     | 0.40              |
| 24:AX:59:A:O2'    | 24:AX:60:U:C5'    | 2.70                     | 0.40              |
| 24:AX:74:C:H2'    | 24:AX:75:C:H5'    | 2.03                     | 0.40              |
| 27:BA:1119:C:H6   | 27:BA:1119:C:O5'  | 2.04                     | 0.40              |
| 27:BA:126:A:C5    | 27:BA:127:A:C6    | 3.09                     | 0.40              |
| 27:BA:1452:A:O3'  | 40:BR:77:ARG:NH1  | 2.54                     | 0.40              |
| 27:BA:1567:A:OP2  | 30:BD:84:TYR:OH   | 2.29                     | 0.40              |
| 27:BA:1591:G:C4   | 27:BA:1592:C:C5   | 3.10                     | 0.40              |
| 27:BA:1861:G:C2   | 27:BA:1862:G:C8   | 3.09                     | 0.40              |
| 27:BA:1998:G:H2'  | 27:BA:1999:C:H6   | 1.85                     | 0.40              |
| 27:BA:2070:G:N1   | 27:BA:2071:A:C2   | 2.90                     | 0.40              |
| 27:BA:2106:G:C2   | 27:BA:2184:G:C2   | 3.09                     | 0.40              |
| 27:BA:2110:G:C5   | 27:BA:2120:G:C8   | 3.10                     | 0.40              |
| 27:BA:2126:A:C5'  | 29:BC:36:LYS:HG2  | 2.52                     | 0.40              |
| 27:BA:2187:G:C6   | 27:BA:2188:C:N3   | 2.90                     | 0.40              |
| 27:BA:2193:G:H2'  | 27:BA:2194:G:H8   | 1.87                     | 0.40              |
| 27:BA:2197:U:O2'  | 27:BA:2198:A:OP2  | 2.32                     | 0.40              |
| 27:BA:2199:A:H8   | 27:BA:2199:A:C5'  | 2.30                     | 0.40              |
| 27:BA:2203:U:H2'  | 27:BA:2205:C:C6   | 2.56                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2259:G:O5'  | 27:BA:2259:G:H8    | 2.03                     | 0.40              |
| 27:BA:2261:C:P    | 49:B0:17:GLN:OE1   | 2.79                     | 0.40              |
| 27:BA:2292:C:C2'  | 27:BA:2293:C:H5'   | 2.52                     | 0.40              |
| 27:BA:2534:A:C2'  | 27:BA:2535:G:O5'   | 2.69                     | 0.40              |
| 27:BA:2652:C:H5'  | 27:BA:2653:U:OP2   | 2.20                     | 0.40              |
| 27:BA:271(P):C:C6 | 27:BA:271(P):C:H5' | 2.49                     | 0.40              |
| 27:BA:2813:A:C2   | 27:BA:2888:C:O2    | 2.74                     | 0.40              |
| 27:BA:2861:G:H2'  | 27:BA:2862:G:H8    | 1.85                     | 0.40              |
| 27:BA:372:G:HO2'  | 27:BA:373:U:P      | 2.44                     | 0.40              |
| 27:BA:45:C:H2'    | 27:BA:47:C:H6      | 1.83                     | 0.40              |
| 27:BA:552:G:C6    | 27:BA:553:G:N7     | 2.89                     | 0.40              |
| 27:BA:729:G:OP2   | 30:BD:13:ARG:HD2   | 2.21                     | 0.40              |
| 27:BA:731:C:O2'   | 27:BA:732:C:H5'    | 2.20                     | 0.40              |
| 27:BA:754:C:C2'   | 27:BA:755:C:O5'    | 2.70                     | 0.40              |
| 27:BA:921:G:H4'   | 27:BA:2269:A:C5    | 2.56                     | 0.40              |
| 29:BC:147:PHE:O   | 29:BC:148:ASN:CB   | 2.69                     | 0.40              |
| 27:BA:606:U:OP1   | 32:BF:104:LYS:HD2  | 2.22                     | 0.40              |
| 33:BG:148:MET:HA  | 33:BG:148:MET:HE3  | 2.03                     | 0.40              |
| 33:BG:148:MET:HG3 | 33:BG:148:MET:O    | 2.20                     | 0.40              |
| 37:BO:97:ARG:CB   | 37:BO:99:PHE:CE1   | 3.03                     | 0.40              |
| 39:BQ:109:VAL:CG1 | 39:BQ:110:THR:N    | 2.84                     | 0.40              |
| 40:BR:23:ASN:H    | 40:BR:23:ASN:ND2   | 2.13                     | 0.40              |
| 41:BS:26:LEU:HA   | 41:BS:39:ILE:HG12  | 2.02                     | 0.40              |
| 46:BX:41:ASN:H    | 46:BX:41:ASN:HD22  | 1.69                     | 0.40              |
| 48:BZ:99:VAL:HA   | 48:BZ:100:PRO:HD3  | 1.90                     | 0.40              |
| 48:BZ:11:GLY:C    | 48:BZ:12:GLU:CD    | 2.80                     | 0.40              |
| 48:BZ:52:ILE:HG22 | 48:BZ:70:VAL:HB    | 1.95                     | 0.40              |
| 1:CA:1315:U:C4    | 1:CA:1316:G:C4     | 3.09                     | 0.40              |
| 1:CA:937:A:H1'    | 1:CA:1379:G:N2     | 2.36                     | 0.40              |
| 1:CA:145:G:C2     | 1:CA:146:G:H1'     | 2.56                     | 0.40              |
| 1:CA:238:G:O2'    | 1:CA:239:U:H5'     | 2.21                     | 0.40              |
| 1:CA:482:A:H2'    | 1:CA:483:C:O4'     | 2.21                     | 0.40              |
| 1:CA:543:C:O2'    | 1:CA:544:G:H5'     | 2.21                     | 0.40              |
| 1:CA:557:G:H3'    | 1:CA:558:G:H8      | 1.86                     | 0.40              |
| 1:CA:570:G:C2     | 1:CA:571:U:C5      | 3.09                     | 0.40              |
| 1:CA:578:C:O2     | 1:CA:579:G:N9      | 2.54                     | 0.40              |
| 1:CA:764:C:C2     | 1:CA:765:G:C8      | 3.09                     | 0.40              |
| 2:CB:17:PHE:N     | 2:CB:17:PHE:CD2    | 2.89                     | 0.40              |
| 1:CA:9:G:OP2      | 5:CE:121:LYS:HD2   | 2.21                     | 0.40              |
| 6:CF:27:GLN:HB3   | 6:CF:27:GLN:HE21   | 1.61                     | 0.40              |
| 7:CG:143:ARG:O    | 7:CG:144:MET:C     | 2.60                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:CG:5:ARG:C       | 7:CG:7:ALA:H       | 2.25                     | 0.40              |
| 7:CG:94:ARG:HB2    | 7:CG:94:ARG:HE     | 1.51                     | 0.40              |
| 8:CH:112:LEU:HD12  | 8:CH:114:THR:CG2   | 2.51                     | 0.40              |
| 9:CI:3:GLN:HA      | 9:CI:20:ARG:HH12   | 1.86                     | 0.40              |
| 1:CA:1278:U:H5     | 10:CJ:99:LYS:HZ3   | 1.70                     | 0.40              |
| 12:CL:42:PRO:HB2   | 12:CL:89:ASP:OD2   | 2.21                     | 0.40              |
| 14:CN:24:CYS:H     | 14:CN:33:VAL:CG1   | 2.33                     | 0.40              |
| 14:CN:41:ARG:HG2   | 14:CN:41:ARG:NH1   | 2.36                     | 0.40              |
| 18:CR:76:LEU:H     | 18:CR:76:LEU:HD22  | 1.86                     | 0.40              |
| 25:CY:58:A:O2'     | 25:CY:59:U:H5'     | 2.21                     | 0.40              |
| 52:D3:22:ALA:HB3   | 52:D3:23:LEU:HD12  | 2.03                     | 0.40              |
| 54:D5:45:VAL:O     | 54:D5:45:VAL:HG12  | 2.20                     | 0.40              |
| 27:DA:242:G:C5'    | 57:D8:62:LEU:HD13  | 2.22                     | 0.40              |
| 27:DA:1171:G:C6    | 27:DA:1173:G:O2'   | 2.74                     | 0.40              |
| 27:DA:1229:G:C2    | 27:DA:1230:C:C2    | 3.10                     | 0.40              |
| 27:DA:1352:U:H3    | 27:DA:1378:A:N6    | 2.12                     | 0.40              |
| 27:DA:1355:G:C6    | 27:DA:1356:G:C5    | 3.09                     | 0.40              |
| 27:DA:142(A):C:C2' | 27:DA:143:G:H5'    | 2.51                     | 0.40              |
| 27:DA:1447:G:C6    | 27:DA:1448:G:C6    | 3.09                     | 0.40              |
| 27:DA:1565:C:H3'   | 30:DD:21:PHE:CZ    | 2.56                     | 0.40              |
| 27:DA:1340:U:C2    | 27:DA:1603:A:H8    | 2.39                     | 0.40              |
| 27:DA:191:A:O2'    | 27:DA:192:C:H5'    | 2.20                     | 0.40              |
| 27:DA:2352:A:C6    | 27:DA:2366:A:C4    | 3.09                     | 0.40              |
| 27:DA:242:G:O2'    | 27:DA:243:U:P      | 2.79                     | 0.40              |
| 27:DA:2445:G:C2'   | 27:DA:2446:G:O5'   | 2.69                     | 0.40              |
| 27:DA:2517:C:H2'   | 27:DA:2542:A:C2    | 2.55                     | 0.40              |
| 27:DA:2536:G:H2'   | 27:DA:2537:U:H6    | 1.85                     | 0.40              |
| 27:DA:2601:C:C2'   | 27:DA:2602:A:OP2   | 2.69                     | 0.40              |
| 27:DA:9:U:O4       | 27:DA:2629:A:N7    | 2.55                     | 0.40              |
| 27:DA:389:G:O5'    | 27:DA:389:G:C8     | 2.71                     | 0.40              |
| 27:DA:403:U:H4'    | 27:DA:404:C:H5'    | 2.03                     | 0.40              |
| 27:DA:596:G:H2'    | 27:DA:597:U:C6     | 2.56                     | 0.40              |
| 28:DB:57:A:H8      | 28:DB:57:A:O5'     | 2.04                     | 0.40              |
| 30:DD:228:PRO:HD3  | 30:DD:235:GLY:CA   | 2.51                     | 0.40              |
| 30:DD:242:ARG:HG2  | 30:DD:246:PRO:HG3  | 2.03                     | 0.40              |
| 27:DA:1845:G:OP1   | 30:DD:258:LYS:HD2  | 2.21                     | 0.40              |
| 31:DE:112:GLY:O    | 31:DE:114:ALA:N    | 2.55                     | 0.40              |
| 31:DE:168:MET:CE   | 31:DE:202:LYS:HE2  | 2.51                     | 0.40              |
| 31:DE:81:ILE:HG21  | 31:DE:84:PHE:HD1   | 1.86                     | 0.40              |
| 32:DF:196:LEU:HA   | 32:DF:196:LEU:HD23 | 1.81                     | 0.40              |
| 34:DH:113:VAL:HG21 | 34:DH:151:ILE:HG21 | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:DI:2:LYS:O     | 35:DI:39:ALA:HB2  | 2.21                     | 0.40              |
| 36:DN:85:ILE:O    | 36:DN:85:ILE:CG2  | 2.69                     | 0.40              |
| 39:DQ:32:TYR:O    | 39:DQ:105:GLU:HA  | 2.21                     | 0.40              |
| 41:DS:78:LEU:C    | 41:DS:80:LEU:N    | 2.74                     | 0.40              |
| 41:DS:97:ARG:CZ   | 41:DS:97:ARG:C    | 2.90                     | 0.40              |
| 42:DT:120:ARG:O   | 42:DT:124:ASP:OD1 | 2.39                     | 0.40              |
| 31:DE:14:ILE:HD12 | 42:DT:14:TYR:CE2  | 2.56                     | 0.40              |
| 43:DU:39:LEU:O    | 43:DU:42:ALA:N    | 2.54                     | 0.40              |
| 43:DU:60:LEU:HA   | 43:DU:63:VAL:CG2  | 2.51                     | 0.40              |
| 45:DW:20:VAL:C    | 45:DW:22:ASP:N    | 2.74                     | 0.40              |
| 46:DX:14:SER:O    | 46:DX:15:GLU:C    | 2.59                     | 0.40              |
| 48:DZ:157:PRO:O   | 48:DZ:160:VAL:HB  | 2.21                     | 0.40              |
| 48:DZ:3:ARG:HA    | 48:DZ:57:VAL:H    | 1.86                     | 0.40              |
| 1:AA:1127:G:O6    | 1:AA:1145:C:N4    | 2.54                     | 0.40              |
| 1:AA:1333:A:H2'   | 1:AA:1334:G:O5'   | 2.21                     | 0.40              |
| 1:AA:1238:A:OP1   | 1:AA:1335:C:H1'   | 2.21                     | 0.40              |
| 1:AA:1452:C:O2'   | 1:AA:1456:G:N2    | 2.55                     | 0.40              |
| 1:AA:1483:A:C8    | 1:AA:1484:C:C6    | 3.08                     | 0.40              |
| 1:AA:1502:A:H2    | 1:AA:1505:G:H1    | 1.70                     | 0.40              |
| 1:AA:189(J):G:C2  | 1:AA:189(K):U:C2  | 3.09                     | 0.40              |
| 1:AA:203:U:H5'    | 1:AA:204:U:OP1    | 2.21                     | 0.40              |
| 1:AA:222:U:H2'    | 1:AA:222:U:O2     | 2.22                     | 0.40              |
| 1:AA:119:A:C8     | 1:AA:240:C:N4     | 2.89                     | 0.40              |
| 1:AA:259:G:C4     | 1:AA:260:G:C8     | 3.09                     | 0.40              |
| 1:AA:241:C:C2     | 1:AA:286:G:C2     | 3.09                     | 0.40              |
| 1:AA:556:C:H2'    | 1:AA:557:G:H8     | 1.86                     | 0.40              |
| 1:AA:885:G:N2     | 1:AA:886:G:C4     | 2.89                     | 0.40              |
| 2:AB:113:HIS:C    | 2:AB:115:LEU:N    | 2.75                     | 0.40              |
| 2:AB:217:ARG:HA   | 2:AB:217:ARG:HD3  | 1.74                     | 0.40              |
| 2:AB:228:GLY:O    | 2:AB:229:VAL:C    | 2.60                     | 0.40              |
| 2:AB:87:ARG:HE    | 2:AB:233:SER:HB2  | 1.86                     | 0.40              |
| 2:AB:46:LYS:C     | 2:AB:48:MET:N     | 2.74                     | 0.40              |
| 3:AC:119:ARG:HA   | 3:AC:122:GLU:CD   | 2.41                     | 0.40              |
| 3:AC:131:ARG:NH1  | 3:AC:135:LYS:HE3  | 2.35                     | 0.40              |
| 3:AC:142:MET:HA   | 3:AC:146:ALA:HB3  | 2.02                     | 0.40              |
| 4:AD:17:VAL:HG12  | 4:AD:18:LYS:O     | 2.21                     | 0.40              |
| 4:AD:176:LEU:HD12 | 4:AD:182:LYS:O    | 2.22                     | 0.40              |
| 4:AD:23:GLY:HA3   | 4:AD:112:VAL:O    | 2.20                     | 0.40              |
| 4:AD:52:SER:O     | 4:AD:55:ALA:CB    | 2.69                     | 0.40              |
| 4:AD:76:ARG:O     | 4:AD:79:PHE:N     | 2.55                     | 0.40              |
| 6:AF:39:LYS:CG    | 6:AF:40:VAL:N     | 2.85                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:AG:127:ALA:C     | 7:AG:129:GLU:H    | 2.25                     | 0.40              |
| 7:AG:137:LYS:O     | 7:AG:141:VAL:CG2  | 2.66                     | 0.40              |
| 7:AG:71:PRO:HG3    | 7:AG:99:LEU:CD1   | 2.52                     | 0.40              |
| 8:AH:83:ILE:CB     | 8:AH:137:VAL:HG13 | 2.45                     | 0.40              |
| 8:AH:35:ILE:O      | 8:AH:38:ILE:HB    | 2.21                     | 0.40              |
| 9:AI:50:LEU:CA     | 9:AI:53:VAL:HG22  | 2.48                     | 0.40              |
| 13:AM:116:THR:CG2  | 13:AM:117:VAL:H   | 2.34                     | 0.40              |
| 20:AT:30:LYS:C     | 20:AT:32:ALA:N    | 2.75                     | 0.40              |
| 23:AW:14:A:H1'     | 23:AW:21:A:C6     | 2.57                     | 0.40              |
| 50:B1:52:ARG:CG    | 50:B1:53:VAL:H    | 2.14                     | 0.40              |
| 51:B2:13:ALA:HA    | 51:B2:16:LEU:CG   | 2.51                     | 0.40              |
| 27:BA:61:G:N7      | 51:B2:51:ARG:NH2  | 2.68                     | 0.40              |
| 51:B2:28:LYS:O     | 51:B2:53:LEU:CD1  | 2.69                     | 0.40              |
| 55:B6:17:LYS:HB3   | 55:B6:18:ARG:NH1  | 2.36                     | 0.40              |
| 58:B9:24:TYR:CZ    | 58:B9:35:ARG:HD2  | 2.55                     | 0.40              |
| 27:BA:1002:G:C2    | 27:BA:1003:G:H1'  | 2.57                     | 0.40              |
| 27:BA:1443:G:N2    | 27:BA:1549:C:C2   | 2.88                     | 0.40              |
| 27:BA:1594:G:C2    | 27:BA:1595:G:C4   | 3.10                     | 0.40              |
| 27:BA:1794:U:H2'   | 27:BA:1795:C:C6   | 2.56                     | 0.40              |
| 27:BA:1806:C:N4    | 27:BA:1812:A:C6   | 2.90                     | 0.40              |
| 27:BA:217:G:C6     | 27:BA:218:A:C5    | 3.10                     | 0.40              |
| 27:BA:2303:G:N2    | 27:BA:2314:C:C2   | 2.89                     | 0.40              |
| 27:BA:2368:C:O2    | 27:BA:2369:A:C8   | 2.74                     | 0.40              |
| 27:BA:241:A:O3'    | 27:BA:242:G:H4'   | 2.22                     | 0.40              |
| 27:BA:2642:G:O2'   | 27:BA:2643:G:H5'  | 2.20                     | 0.40              |
| 27:BA:2671:A:C2    | 27:BA:2672:G:N3   | 2.90                     | 0.40              |
| 27:BA:271(O):C:O2' | 27:BA:271(P):C:C5 | 2.71                     | 0.40              |
| 27:BA:2746:U:C2'   | 27:BA:2747:G:H5'  | 2.50                     | 0.40              |
| 27:BA:42:G:C6      | 27:BA:43:A:C4     | 3.09                     | 0.40              |
| 27:BA:530:G:C2     | 27:BA:2022:U:OP1  | 2.75                     | 0.40              |
| 27:BA:560:C:H2'    | 27:BA:561:G:O5'   | 2.21                     | 0.40              |
| 27:BA:74:A:HO2'    | 27:BA:88:G:H8     | 1.69                     | 0.40              |
| 27:BA:807:U:H2'    | 27:BA:808:G:O5'   | 2.21                     | 0.40              |
| 27:BA:86:C:H2'     | 27:BA:86:C:O2     | 2.21                     | 0.40              |
| 29:BC:195:ALA:C    | 29:BC:197:GLU:N   | 2.74                     | 0.40              |
| 30:BD:233:HIS:CD2  | 30:BD:233:HIS:N   | 2.90                     | 0.40              |
| 30:BD:35:LYS:HA    | 30:BD:64:ILE:CG2  | 2.48                     | 0.40              |
| 31:BE:117:MET:O    | 31:BE:117:MET:CG  | 2.69                     | 0.40              |
| 32:BF:106:ARG:O    | 32:BF:107:LYS:C   | 2.59                     | 0.40              |
| 32:BF:33:LEU:HA    | 32:BF:33:LEU:HD12 | 1.86                     | 0.40              |
| 32:BF:57:VAL:HG13  | 32:BF:59:TYR:H    | 1.86                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:BF:68:LYS:C     | 32:BF:70:THR:N    | 2.71                     | 0.40              |
| 34:BH:137:ASP:CG   | 34:BH:140:LYS:HB3 | 2.42                     | 0.40              |
| 34:BH:17:VAL:O     | 34:BH:45:VAL:HG22 | 2.20                     | 0.40              |
| 34:BH:54:ARG:HA    | 34:BH:55:PRO:HD2  | 1.79                     | 0.40              |
| 34:BH:61:HIS:O     | 34:BH:64:LEU:N    | 2.42                     | 0.40              |
| 35:BI:116:LEU:HD12 | 35:BI:117:GLU:N   | 2.35                     | 0.40              |
| 35:BI:124:GLY:O    | 35:BI:125:GLU:OE1 | 2.40                     | 0.40              |
| 35:BI:41:GLU:O     | 35:BI:44:LEU:CB   | 2.70                     | 0.40              |
| 38:BP:57:THR:HG1   | 38:BP:59:LEU:HB3  | 1.87                     | 0.40              |
| 38:BP:6:LEU:CD1    | 38:BP:8:PRO:HG2   | 2.50                     | 0.40              |
| 40:BR:81:ASP:O     | 40:BR:82:GLU:HB2  | 2.20                     | 0.40              |
| 43:BU:107:ALA:O    | 43:BU:110:VAL:HB  | 2.22                     | 0.40              |
| 44:BV:14:VAL:O     | 44:BV:15:GLU:HG3  | 2.21                     | 0.40              |
| 44:BV:80:GLN:NE2   | 44:BV:80:GLN:HA   | 2.37                     | 0.40              |
| 46:BX:41:ASN:O     | 46:BX:42:ALA:C    | 2.59                     | 0.40              |
| 47:BY:3:VAL:C      | 47:BY:5:MET:H     | 2.23                     | 0.40              |
| 48:BZ:81:ARG:CZ    | 48:BZ:82:PRO:O    | 2.69                     | 0.40              |
| 1:CA:1076:C:H2'    | 1:CA:1077:G:C8    | 2.56                     | 0.40              |
| 1:CA:1442(A):G:H2' | 1:CA:1442(A):G:N3 | 2.36                     | 0.40              |
| 1:CA:1410:G:C2     | 1:CA:1491:G:C2    | 3.10                     | 0.40              |
| 1:CA:225:C:O2      | 1:CA:225:C:C2'    | 2.64                     | 0.40              |
| 1:CA:28:G:O2'      | 1:CA:296:U:OP1    | 2.40                     | 0.40              |
| 1:CA:392:G:C2      | 1:CA:393:A:C4     | 3.09                     | 0.40              |
| 1:CA:504:C:O4'     | 1:CA:510:A:C6     | 2.74                     | 0.40              |
| 1:CA:606:G:H3'     | 1:CA:607:A:C5'    | 2.50                     | 0.40              |
| 1:CA:690:G:H3'     | 1:CA:691:G:C8     | 2.55                     | 0.40              |
| 1:CA:781:A:H5'     | 1:CA:782:A:OP2    | 2.21                     | 0.40              |
| 1:CA:918:A:C4      | 1:CA:919:A:C8     | 3.09                     | 0.40              |
| 2:CB:85:ALA:HB3    | 2:CB:92:TYR:CD2   | 2.55                     | 0.40              |
| 3:CC:148:GLY:CA    | 3:CC:203:PHE:HB3  | 2.51                     | 0.40              |
| 5:CE:78:HIS:HD2    | 5:CE:79:GLU:O     | 2.03                     | 0.40              |
| 5:CE:82:VAL:O      | 5:CE:89:ILE:HG22  | 2.21                     | 0.40              |
| 6:CF:2:ARG:O       | 6:CF:66:GLU:HG3   | 2.21                     | 0.40              |
| 8:CH:25:ASP:O      | 8:CH:26:VAL:HB    | 2.22                     | 0.40              |
| 2:CB:178:ARG:NH2   | 8:CH:74:PRO:HB3   | 2.36                     | 0.40              |
| 9:CI:15:ALA:HB2    | 9:CI:65:VAL:HB    | 2.03                     | 0.40              |
| 9:CI:42:ARG:O      | 9:CI:74:ILE:HD13  | 2.21                     | 0.40              |
| 11:CK:29:ILE:HD11  | 11:CK:42:TRP:CE3  | 2.57                     | 0.40              |
| 15:CO:42:HIS:CE1   | 15:CO:46:HIS:ND1  | 2.89                     | 0.40              |
| 16:CP:71:ARG:O     | 16:CP:72:ARG:C    | 2.58                     | 0.40              |
| 19:CS:22:LEU:CD1   | 19:CS:27:GLU:HB3  | 2.50                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:CU:24:ARG:NH1  | 21:CU:24:ARG:HG2  | 2.37                     | 0.40              |
| 49:D0:21:LEU:HD23 | 49:D0:39:ARG:HB3  | 2.02                     | 0.40              |
| 51:D2:19:VAL:O    | 51:D2:21:LEU:N    | 2.54                     | 0.40              |
| 52:D3:22:ALA:O    | 52:D3:26:LEU:HG   | 2.21                     | 0.40              |
| 52:D3:7:LYS:NZ    | 52:D3:32:GLN:NE2  | 2.68                     | 0.40              |
| 55:D6:27:LYS:O    | 55:D6:29:ASN:OD1  | 2.39                     | 0.40              |
| 55:D6:43:CYS:O    | 55:D6:44:ARG:O    | 2.40                     | 0.40              |
| 27:DA:54:G:H1'    | 56:D7:35:ARG:HH11 | 1.86                     | 0.40              |
| 57:D8:28:GLY:HA2  | 57:D8:32:LEU:HD21 | 2.03                     | 0.40              |
| 27:DA:1200:C:H2'  | 27:DA:1201:C:H6   | 1.85                     | 0.40              |
| 27:DA:1443:G:C6   | 27:DA:1444:G:C5   | 3.10                     | 0.40              |
| 27:DA:1553:A:C8   | 27:DA:1555:G:C6   | 3.10                     | 0.40              |
| 27:DA:1887:C:H3'  | 27:DA:1888:G:C5'  | 2.46                     | 0.40              |
| 26:CZ:4:SER:O     | 27:DA:1914:C:OP2  | 2.40                     | 0.40              |
| 27:DA:1945:G:O2'  | 27:DA:1946:U:C5'  | 2.69                     | 0.40              |
| 27:DA:1951:U:O2   | 27:DA:1953:A:H8   | 2.04                     | 0.40              |
| 27:DA:1986:A:N3   | 27:DA:1987:G:C8   | 2.90                     | 0.40              |
| 27:DA:2016:U:H2'  | 27:DA:2017:U:H6   | 1.86                     | 0.40              |
| 27:DA:2046:G:C2   | 27:DA:2047:U:C6   | 3.09                     | 0.40              |
| 27:DA:2074:U:O2   | 27:DA:2436:G:C2   | 2.74                     | 0.40              |
| 27:DA:2313:C:C3'  | 27:DA:2313:C:C6   | 3.04                     | 0.40              |
| 27:DA:2347:C:H4'  | 55:D6:39:TYR:HE1  | 1.87                     | 0.40              |
| 27:DA:2467:C:N4   | 27:DA:2468:G:N1   | 2.68                     | 0.40              |
| 27:DA:2470:G:O2'  | 27:DA:2471:C:H5'  | 2.21                     | 0.40              |
| 27:DA:2517:C:C6   | 27:DA:2542:A:C2   | 3.09                     | 0.40              |
| 27:DA:2533:A:H2'  | 27:DA:2534:A:O4'  | 2.20                     | 0.40              |
| 27:DA:2641:G:H4'  | 36:DN:76:SER:HB3  | 2.03                     | 0.40              |
| 27:DA:2844:G:C2   | 27:DA:2874:C:N3   | 2.89                     | 0.40              |
| 27:DA:444:C:H4'   | 32:DF:49:ALA:HB2  | 2.03                     | 0.40              |
| 27:DA:451:C:H41   | 27:DA:453:C:H3'   | 1.86                     | 0.40              |
| 27:DA:52:A:N6     | 27:DA:118:A:N3    | 2.69                     | 0.40              |
| 27:DA:555:U:HO2'  | 27:DA:556:G:H8    | 1.68                     | 0.40              |
| 27:DA:645:C:O2    | 27:DA:645:C:H2'   | 2.20                     | 0.40              |
| 27:DA:599:G:N2    | 27:DA:659:C:C2    | 2.89                     | 0.40              |
| 27:DA:729:G:H5'   | 27:DA:730:C:H5''  | 2.02                     | 0.40              |
| 27:DA:889:C:O2'   | 27:DA:890:A:P     | 2.79                     | 0.40              |
| 30:DD:134:ARG:HD3 | 30:DD:135:PHE:CZ  | 2.57                     | 0.40              |
| 30:DD:263:ARG:O   | 30:DD:264:LYS:C   | 2.60                     | 0.40              |
| 30:DD:31:LYS:HD3  | 30:DD:94:LEU:HD11 | 2.03                     | 0.40              |
| 33:DG:105:LYS:HB3 | 33:DG:142:PRO:HG3 | 2.03                     | 0.40              |
| 35:DI:139:GLN:HG3 | 35:DI:140:LEU:H   | 1.85                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:DI:72:LEU:HD21 | 35:DI:75:LEU:HD23 | 2.03                     | 0.40              |
| 35:DI:88:ILE:HD11 | 35:DI:123:LEU:N   | 2.36                     | 0.40              |
| 36:DN:100:GLU:O   | 36:DN:104:LYS:CB  | 2.70                     | 0.40              |
| 36:DN:24:GLY:O    | 36:DN:28:THR:HG22 | 2.21                     | 0.40              |
| 37:DO:110:GLY:O   | 37:DO:112:MET:N   | 2.55                     | 0.40              |
| 38:DP:65:ARG:O    | 38:DP:68:GLN:OE1  | 2.39                     | 0.40              |
| 39:DQ:132:VAL:HB  | 48:DZ:80:ARG:NH2  | 2.37                     | 0.40              |
| 42:DT:106:SER:HA  | 42:DT:110:ILE:CG1 | 2.50                     | 0.40              |
| 43:DU:33:ARG:O    | 43:DU:36:ARG:N    | 2.52                     | 0.40              |
| 43:DU:6:THR:HG21  | 43:DU:10:ARG:HE   | 1.86                     | 0.40              |
| 1:AA:1047:G:O2'   | 1:AA:1215:G:O2'   | 2.25                     | 0.40              |
| 1:AA:1173:G:C5    | 1:AA:1174:G:N7    | 2.89                     | 0.40              |
| 1:AA:1295:G:C6    | 1:AA:1296:C:C4    | 3.09                     | 0.40              |
| 1:AA:1316:G:N2    | 1:AA:1319:A:OP2   | 2.53                     | 0.40              |
| 1:AA:1330:U:OP1   | 13:AM:25:ILE:O    | 2.40                     | 0.40              |
| 1:AA:1401:G:O2'   | 1:AA:1402:C:H5'   | 2.21                     | 0.40              |
| 1:AA:169:C:H2'    | 1:AA:170:U:H6     | 1.85                     | 0.40              |
| 1:AA:218:C:H2'    | 1:AA:219:C:O4'    | 2.21                     | 0.40              |
| 1:AA:268:C:H2'    | 1:AA:269:C:H6     | 1.86                     | 0.40              |
| 1:AA:506:G:H2'    | 1:AA:507:C:C6     | 2.56                     | 0.40              |
| 1:AA:592:G:C2     | 1:AA:593:G:N7     | 2.90                     | 0.40              |
| 1:AA:577:G:C6     | 1:AA:765:G:C2     | 3.09                     | 0.40              |
| 1:AA:953:G:O6     | 13:AM:104:ARG:HD2 | 2.21                     | 0.40              |
| 1:AA:9:G:H5'      | 5:AE:122:GLU:CD   | 2.42                     | 0.40              |
| 2:AB:44:LEU:O     | 2:AB:47:THR:HB    | 2.20                     | 0.40              |
| 2:AB:97:TRP:CH2   | 2:AB:176:GLU:OE2  | 2.75                     | 0.40              |
| 1:AA:1060:C:C4    | 3:AC:2:GLY:HA2    | 2.57                     | 0.40              |
| 3:AC:42:LEU:HA    | 3:AC:45:LYS:HG3   | 2.03                     | 0.40              |
| 5:AE:32:VAL:CG2   | 5:AE:58:ALA:HB3   | 2.52                     | 0.40              |
| 8:AH:34:GLU:OE1   | 8:AH:34:GLU:HA    | 2.21                     | 0.40              |
| 11:AK:88:GLY:C    | 11:AK:90:GLY:N    | 2.74                     | 0.40              |
| 15:AO:5:LYS:HA    | 15:AO:8:LYS:CB    | 2.50                     | 0.40              |
| 19:AS:37:ARG:C    | 19:AS:37:ARG:HD3  | 2.41                     | 0.40              |
| 19:AS:41:VAL:HA   | 19:AS:42:PRO:HD3  | 1.88                     | 0.40              |
| 20:AT:44:ALA:O    | 20:AT:92:LEU:HD23 | 2.21                     | 0.40              |
| 20:AT:59:ALA:C    | 20:AT:61:SER:N    | 2.74                     | 0.40              |
| 23:AW:58:A:H2'    | 23:AW:59:U:O4'    | 2.21                     | 0.40              |
| 49:B0:65:GLY:CA   | 49:B0:83:PRO:HA   | 2.46                     | 0.40              |
| 52:B3:3:ARG:HB3   | 52:B3:59:VAL:HB   | 2.03                     | 0.40              |
| 54:B5:18:ALA:C    | 54:B5:20:ARG:N    | 2.69                     | 0.40              |
| 27:BA:1346:G:N3   | 27:BA:1347:G:C8   | 2.88                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BA:1481:U:C2'   | 27:BA:1481:U:O2    | 2.62                     | 0.40              |
| 27:BA:1505:C:H3'   | 27:BA:1506:C:C5    | 2.56                     | 0.40              |
| 27:BA:1707:G:C8    | 27:BA:1707:G:OP2   | 2.73                     | 0.40              |
| 27:BA:1905:C:H1'   | 27:BA:1928:A:C2    | 2.57                     | 0.40              |
| 27:BA:206:U:O2'    | 27:BA:207:A:H5'    | 2.22                     | 0.40              |
| 27:BA:2072:G:C6    | 27:BA:2073:C:C4    | 3.09                     | 0.40              |
| 27:BA:2228:G:C5    | 27:BA:2229:C:C4    | 3.09                     | 0.40              |
| 27:BA:2402:C:C3'   | 27:BA:2403:C:H5'   | 2.51                     | 0.40              |
| 27:BA:240:G:C6     | 27:BA:241:A:N6     | 2.90                     | 0.40              |
| 25:AY:75:A:N6      | 27:BA:2422:A:O4'   | 2.55                     | 0.40              |
| 27:BA:271(R):G:H2' | 27:BA:271(S):G:C8  | 2.57                     | 0.40              |
| 27:BA:2842:G:C6    | 27:BA:2876:G:N1    | 2.89                     | 0.40              |
| 27:BA:363(B):G:H5' | 27:BA:363(C):G:OP2 | 2.22                     | 0.40              |
| 27:BA:569:U:H2'    | 27:BA:570:G:O4'    | 2.21                     | 0.40              |
| 27:BA:681:G:H2'    | 27:BA:682:G:C8     | 2.54                     | 0.40              |
| 27:BA:791:C:H4'    | 27:BA:792:G:OP1    | 2.21                     | 0.40              |
| 27:BA:807:U:C2'    | 27:BA:808:G:C5'    | 2.99                     | 0.40              |
| 27:BA:866:A:O2'    | 27:BA:867:C:H5'    | 2.21                     | 0.40              |
| 29:BC:134:ARG:O    | 29:BC:136:LEU:N    | 2.42                     | 0.40              |
| 30:BD:146:GLU:HB3  | 30:BD:189:CYS:HB3  | 2.04                     | 0.40              |
| 31:BE:120:TRP:CG   | 31:BE:155:LYS:HB3  | 2.56                     | 0.40              |
| 31:BE:47:VAL:HB    | 31:BE:49:LEU:HD11  | 2.02                     | 0.40              |
| 32:BF:127:GLU:HG2  | 32:BF:196:LEU:HD12 | 2.04                     | 0.40              |
| 32:BF:191:ARG:HH11 | 32:BF:191:ARG:HG2  | 1.86                     | 0.40              |
| 33:BG:63:ILE:HG12  | 33:BG:63:ILE:H     | 1.66                     | 0.40              |
| 35:BI:116:LEU:HD12 | 35:BI:117:GLU:H    | 1.86                     | 0.40              |
| 36:BN:35:ARG:C     | 36:BN:37:LYS:N     | 2.74                     | 0.40              |
| 37:BO:2:ILE:HG12   | 37:BO:33:ALA:O     | 2.21                     | 0.40              |
| 37:BO:38:VAL:C     | 37:BO:39:ILE:HG23  | 2.42                     | 0.40              |
| 37:BO:22:ILE:CG1   | 37:BO:41:ALA:HA    | 2.35                     | 0.40              |
| 38:BP:81:GLN:OE1   | 38:BP:106:LEU:CA   | 2.70                     | 0.40              |
| 27:BA:251:A:C5'    | 38:BP:51:PHE:HZ    | 2.34                     | 0.40              |
| 38:BP:71:VAL:HG13  | 38:BP:72:PRO:N     | 2.37                     | 0.40              |
| 39:BQ:52:VAL:HG13  | 39:BQ:56:ARG:HG3   | 2.03                     | 0.40              |
| 40:BR:5:LYS:HD2    | 40:BR:5:LYS:N      | 2.37                     | 0.40              |
| 41:BS:103:GLU:CD   | 41:BS:103:GLU:N    | 2.74                     | 0.40              |
| 41:BS:106:ARG:O    | 41:BS:106:ARG:HG2  | 2.21                     | 0.40              |
| 42:BT:46:GLU:HG3   | 42:BT:47:GLY:N     | 2.36                     | 0.40              |
| 43:BU:31:SER:HG    | 43:BU:34:LYS:N     | 2.17                     | 0.40              |
| 45:BW:68:ARG:O     | 45:BW:110:LYS:N    | 2.54                     | 0.40              |
| 46:BX:5:TYR:HD1    | 51:B2:29:LYS:HB2   | 1.87                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:BY:79:CYS:SG   | 47:BY:80:GLY:N    | 2.94                     | 0.40              |
| 1:CA:1066:C:C5'   | 1:CA:1066:C:C6    | 2.88                     | 0.40              |
| 1:CA:109:A:H2'    | 1:CA:326:G:H21    | 1.87                     | 0.40              |
| 1:CA:112:G:HO2'   | 1:CA:354:G:HO2'   | 1.66                     | 0.40              |
| 1:CA:1198:G:C6    | 1:CA:1199:U:C4    | 3.10                     | 0.40              |
| 1:CA:1253:G:H5'   | 10:CJ:44:VAL:O    | 2.21                     | 0.40              |
| 1:CA:1305:G:OP2   | 1:CA:1305:G:C8    | 2.75                     | 0.40              |
| 1:CA:1308:U:O3'   | 13:CM:92:HIS:CE1  | 2.74                     | 0.40              |
| 1:CA:1328:C:P     | 21:CU:21:TYR:HH   | 2.44                     | 0.40              |
| 1:CA:1523:G:C5    | 1:CA:1524:C:C4    | 3.10                     | 0.40              |
| 1:CA:270:A:C6     | 1:CA:271:C:C4     | 3.09                     | 0.40              |
| 1:CA:321:A:O2'    | 1:CA:322:C:C5'    | 2.64                     | 0.40              |
| 1:CA:332:G:C4     | 1:CA:333:G:C8     | 3.09                     | 0.40              |
| 1:CA:600:C:N3     | 1:CA:639:G:C2     | 2.90                     | 0.40              |
| 1:CA:866:C:C5     | 1:CA:867:G:H1'    | 2.55                     | 0.40              |
| 3:CC:119:ARG:HE   | 3:CC:140:ARG:NE   | 2.19                     | 0.40              |
| 4:CD:165:MET:SD   | 4:CD:168:ARG:HD3  | 2.61                     | 0.40              |
| 4:CD:108:LEU:CD1  | 4:CD:174:LEU:HD13 | 2.51                     | 0.40              |
| 9:CI:29:ASN:OD1   | 9:CI:64:THR:HA    | 2.21                     | 0.40              |
| 10:CJ:13:HIS:HB3  | 10:CJ:68:HIS:NE2  | 2.36                     | 0.40              |
| 10:CJ:4:ILE:HB    | 10:CJ:74:ILE:HG13 | 2.02                     | 0.40              |
| 12:CL:82:ILE:HD13 | 12:CL:82:ILE:HA   | 1.85                     | 0.40              |
| 13:CM:23:TYR:HE1  | 13:CM:71:ARG:HA   | 1.87                     | 0.40              |
| 13:CM:80:ARG:C    | 13:CM:82:MET:N    | 2.75                     | 0.40              |
| 14:CN:15:LYS:HB3  | 14:CN:16:PHE:CD2  | 2.57                     | 0.40              |
| 14:CN:21:TYR:CD2  | 14:CN:22:THR:O    | 2.72                     | 0.40              |
| 1:CA:238:G:P      | 17:CQ:25:ARG:HH22 | 2.43                     | 0.40              |
| 17:CQ:31:LEU:HD23 | 17:CQ:32:TYR:CE2  | 2.56                     | 0.40              |
| 18:CR:46:GLU:HA   | 18:CR:46:GLU:OE2  | 2.22                     | 0.40              |
| 23:CW:47:C:C2     | 23:CW:58:A:H1'    | 2.56                     | 0.40              |
| 24:CX:61:C:O2'    | 24:CX:62:C:P      | 2.79                     | 0.40              |
| 49:D0:19:LYS:O    | 49:D0:20:ARG:C    | 2.59                     | 0.40              |
| 50:D1:47:GLN:HE21 | 50:D1:47:GLN:CA   | 2.34                     | 0.40              |
| 53:D4:43:GLY:H    | 53:D4:59:VAL:HG12 | 1.86                     | 0.40              |
| 56:D7:14:LYS:HG2  | 56:D7:14:LYS:H    | 1.67                     | 0.40              |
| 57:D8:17:THR:HG23 | 57:D8:23:VAL:CG2  | 2.51                     | 0.40              |
| 27:DA:1158:C:O2'  | 27:DA:1159:U:C5'  | 2.61                     | 0.40              |
| 27:DA:1525:G:H2'  | 27:DA:1526:G:C8   | 2.56                     | 0.40              |
| 27:DA:1560:G:H5'  | 27:DA:1560:G:H8   | 1.86                     | 0.40              |
| 27:DA:1576:U:H2'  | 27:DA:1577:C:H6   | 1.87                     | 0.40              |
| 27:DA:1750:G:H2'  | 27:DA:1751:C:C6   | 2.57                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DA:1752:C:H2'  | 27:DA:1753:G:C8    | 2.57                     | 0.40              |
| 27:DA:1790:C:H2'  | 27:DA:1791:A:C4    | 2.56                     | 0.40              |
| 27:DA:1819:A:C5'  | 30:DD:158:ALA:CB   | 2.95                     | 0.40              |
| 27:DA:1836:C:H2'  | 27:DA:1836:C:O2    | 2.21                     | 0.40              |
| 27:DA:1856:G:C2   | 27:DA:1857:G:H1'   | 2.57                     | 0.40              |
| 27:DA:1855:G:O2'  | 27:DA:1856:G:H5'   | 2.21                     | 0.40              |
| 27:DA:2258:C:C2'  | 27:DA:2426:A:H4'   | 2.52                     | 0.40              |
| 27:DA:2302:G:N3   | 27:DA:2302:G:H2'   | 2.36                     | 0.40              |
| 27:DA:2495:G:C2   | 27:DA:2496:C:C2    | 3.10                     | 0.40              |
| 27:DA:2554:U:H2'  | 27:DA:2555:U:H6    | 1.87                     | 0.40              |
| 27:DA:2561:A:C2   | 27:DA:2562:U:C6    | 3.10                     | 0.40              |
| 27:DA:1629:U:O2'  | 27:DA:2698:U:OP1   | 2.39                     | 0.40              |
| 27:DA:2848:G:O2'  | 27:DA:2867:G:N1    | 2.35                     | 0.40              |
| 27:DA:2854:G:C2   | 27:DA:2864:G:C2    | 3.10                     | 0.40              |
| 27:DA:405:U:HO2'  | 27:DA:406:G:P      | 2.45                     | 0.40              |
| 27:DA:660:G:C6    | 27:DA:661:C:C2     | 3.10                     | 0.40              |
| 27:DA:675:A:O2'   | 32:DF:67:GLN:NE2   | 2.55                     | 0.40              |
| 27:DA:864:G:C4    | 27:DA:865:C:H5     | 2.39                     | 0.40              |
| 27:DA:869:G:C4    | 27:DA:870:A:N7     | 2.90                     | 0.40              |
| 27:DA:969:U:OP1   | 52:D3:17:LYS:CG    | 2.58                     | 0.40              |
| 29:DC:62:VAL:O    | 29:DC:63:SER:C     | 2.60                     | 0.40              |
| 30:DD:174:ILE:C   | 30:DD:175:LEU:HD23 | 2.40                     | 0.40              |
| 30:DD:40:THR:O    | 30:DD:41:GLY:C     | 2.56                     | 0.40              |
| 31:DE:15:PHE:CZ   | 42:DT:80:SER:CB    | 3.04                     | 0.40              |
| 31:DE:81:ILE:O    | 31:DE:82:ARG:CB    | 2.66                     | 0.40              |
| 34:DH:122:THR:HB  | 34:DH:134:SER:HB2  | 2.04                     | 0.40              |
| 34:DH:147:ASN:H   | 34:DH:147:ASN:HD22 | 1.57                     | 0.40              |
| 34:DH:160:LYS:HG3 | 34:DH:160:LYS:H    | 1.70                     | 0.40              |
| 36:DN:74:ARG:O    | 36:DN:82:LEU:HA    | 2.21                     | 0.40              |
| 36:DN:89:LYS:C    | 36:DN:89:LYS:HZ3   | 2.25                     | 0.40              |
| 37:DO:16:ALA:HB1  | 37:DO:43:VAL:CG1   | 2.52                     | 0.40              |
| 39:DQ:55:VAL:O    | 39:DQ:56:ARG:C     | 2.59                     | 0.40              |
| 40:DR:103:ARG:HB3 | 40:DR:109:ALA:O    | 2.21                     | 0.40              |
| 40:DR:59:ASP:O    | 40:DR:62:ALA:HB3   | 2.21                     | 0.40              |
| 42:DT:118:ARG:C   | 42:DT:120:ARG:N    | 2.70                     | 0.40              |
| 42:DT:62:THR:HG22 | 42:DT:75:ILE:HG13  | 2.03                     | 0.40              |
| 43:DU:104:GLN:O   | 43:DU:105:VAL:C    | 2.60                     | 0.40              |
| 27:DA:581:C:OP1   | 43:DU:31:SER:OG    | 2.40                     | 0.40              |
| 43:DU:67:ALA:HA   | 43:DU:70:ARG:HB2   | 2.04                     | 0.40              |
| 43:DU:80:ILE:HA   | 43:DU:83:LEU:HB2   | 2.03                     | 0.40              |
| 44:DV:2:PHE:CB    | 44:DV:42:GLY:CA    | 2.91                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:DW:20:VAL:O    | 45:DW:23:LEU:HB2  | 2.21                     | 0.40              |
| 47:DY:17:SER:HB2  | 47:DY:71:LYS:HB3  | 2.02                     | 0.40              |
| 47:DY:50:ARG:NH2  | 47:DY:55:TYR:HE1  | 2.19                     | 0.40              |
| 47:DY:84:ARG:HB3  | 47:DY:85:VAL:H    | 1.74                     | 0.40              |
| 48:DZ:102:ARG:HD3 | 48:DZ:135:PHE:CD1 | 2.57                     | 0.40              |
| 48:DZ:144:GLU:HB3 | 48:DZ:145:ILE:H   | 1.52                     | 0.40              |
| 1:AA:996:A:C2     | 1:AA:1046:A:H4'   | 2.56                     | 0.40              |
| 1:AA:1056:U:O2'   | 1:AA:1057:G:H5'   | 2.22                     | 0.40              |
| 1:AA:1164:G:N1    | 1:AA:1173:G:C6    | 2.90                     | 0.40              |
| 1:AA:1279:A:N3    | 1:AA:1279:A:H3'   | 2.36                     | 0.40              |
| 1:AA:1342:C:H2'   | 1:AA:1343:G:H8    | 1.86                     | 0.40              |
| 1:AA:1347:G:HO2'  | 1:AA:1348:U:P     | 2.41                     | 0.40              |
| 1:AA:1351:U:H2'   | 1:AA:1352:C:H6    | 1.87                     | 0.40              |
| 1:AA:441:A:N6     | 1:AA:494:U:C6     | 2.89                     | 0.40              |
| 1:AA:930:C:O2'    | 1:AA:931:C:H5'    | 2.21                     | 0.40              |
| 2:AB:209:ARG:O    | 2:AB:210:SER:C    | 2.59                     | 0.40              |
| 3:AC:122:GLU:O    | 3:AC:126:ARG:HG3  | 2.22                     | 0.40              |
| 5:AE:146:ALA:O    | 5:AE:147:ASP:C    | 2.60                     | 0.40              |
| 5:AE:31:LEU:HD23  | 5:AE:31:LEU:HA    | 1.87                     | 0.40              |
| 1:AA:738:C:H5'    | 6:AF:72:VAL:HG11  | 2.02                     | 0.40              |
| 7:AG:115:ARG:CB   | 7:AG:118:VAL:HG13 | 2.51                     | 0.40              |
| 8:AH:32:LYS:HA    | 8:AH:35:ILE:CD1   | 2.47                     | 0.40              |
| 8:AH:6:ILE:HB     | 8:AH:85:ARG:NH2   | 2.36                     | 0.40              |
| 1:AA:1199:U:C4'   | 10:AJ:54:PHE:CE2  | 3.05                     | 0.40              |
| 10:AJ:33:GLN:O    | 10:AJ:75:ILE:HG12 | 2.20                     | 0.40              |
| 11:AK:65:ALA:O    | 11:AK:66:LEU:C    | 2.59                     | 0.40              |
| 12:AL:55:VAL:CG1  | 12:AL:56:ARG:N    | 2.85                     | 0.40              |
| 12:AL:2:PRO:CA    | 12:AL:6:GLN:HE21  | 2.34                     | 0.40              |
| 13:AM:89:GLY:C    | 13:AM:90:LEU:O    | 2.55                     | 0.40              |
| 3:AC:6:HIS:ND1    | 14:AN:49:HIS:HB3  | 2.37                     | 0.40              |
| 15:AO:35:ARG:HH12 | 15:AO:59:MET:CE   | 2.34                     | 0.40              |
| 20:AT:22:ARG:O    | 20:AT:23:ARG:C    | 2.60                     | 0.40              |
| 49:B0:17:GLN:O    | 49:B0:18:ALA:C    | 2.59                     | 0.40              |
| 27:BA:2271:G:OP1  | 49:B0:20:ARG:HA   | 2.22                     | 0.40              |
| 52:B3:17:LYS:O    | 52:B3:20:LYS:N    | 2.55                     | 0.40              |
| 54:B5:31:VAL:HB   | 54:B5:32:PRO:CD   | 2.50                     | 0.40              |
| 55:B6:4:GLU:O     | 55:B6:5:VAL:C     | 2.60                     | 0.40              |
| 58:B9:17:ILE:HD13 | 58:B9:17:ILE:HA   | 1.93                     | 0.40              |
| 27:BA:107:C:C4    | 27:BA:108:U:H5    | 2.39                     | 0.40              |
| 27:BA:1424:G:H2'  | 27:BA:1425:G:O4'  | 2.21                     | 0.40              |
| 27:BA:173:G:N2    | 27:BA:174:C:C2    | 2.89                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BA:2048:G:N1   | 27:BA:2621:A:C2    | 2.89                     | 0.40              |
| 27:BA:2188:C:H2'  | 27:BA:2189:U:O4'   | 2.20                     | 0.40              |
| 27:BA:2353:G:C6   | 27:BA:2365:G:N2    | 2.89                     | 0.40              |
| 27:BA:2525:G:N2   | 27:BA:2526:G:C4    | 2.89                     | 0.40              |
| 27:BA:2579:C:H2'  | 27:BA:2580:U:O4'   | 2.22                     | 0.40              |
| 27:BA:2765:A:C3'  | 27:BA:2766:G:H5'   | 2.52                     | 0.40              |
| 27:BA:30:G:C6     | 27:BA:31:C:N4      | 2.89                     | 0.40              |
| 27:BA:56:A:H2'    | 27:BA:57:C:C6      | 2.56                     | 0.40              |
| 30:BD:68:LYS:HB2  | 30:BD:68:LYS:HE3   | 1.79                     | 0.40              |
| 30:BD:68:LYS:HE3  | 30:BD:70:TRP:NE1   | 2.37                     | 0.40              |
| 30:BD:85:ASP:OD2  | 30:BD:92:ILE:HG21  | 2.21                     | 0.40              |
| 27:BA:744:G:P     | 31:BE:132:HIS:HB3  | 2.60                     | 0.40              |
| 33:BG:140:ILE:H   | 33:BG:140:ILE:HG13 | 1.69                     | 0.40              |
| 35:BI:110:ASP:HA  | 35:BI:111:PRO:HD2  | 1.87                     | 0.40              |
| 35:BI:79:ILE:HG22 | 35:BI:81:VAL:HG22  | 2.03                     | 0.40              |
| 38:BP:100:LEU:O   | 38:BP:105:LEU:O    | 2.40                     | 0.40              |
| 38:BP:111:ARG:CZ  | 38:BP:149:GLU:HG3  | 2.51                     | 0.40              |
| 38:BP:90:ARG:HB2  | 38:BP:90:ARG:HE    | 1.57                     | 0.40              |
| 42:BT:82:LEU:O    | 42:BT:83:ILE:O     | 2.40                     | 0.40              |
| 44:BV:21:ARG:HG3  | 44:BV:93:GLU:HG3   | 2.02                     | 0.40              |
| 45:BW:12:ILE:HG12 | 45:BW:13:SER:N     | 2.37                     | 0.40              |
| 45:BW:13:SER:HA   | 45:BW:14:PRO:HD3   | 2.00                     | 0.40              |
| 47:BY:46:LYS:HE2  | 47:BY:47:LYS:CE    | 2.49                     | 0.40              |
| 47:BY:61:ILE:O    | 47:BY:62:GLU:O     | 2.39                     | 0.40              |
| 48:BZ:33:ASN:O    | 48:BZ:34:ARG:C     | 2.60                     | 0.40              |
| 1:CA:1154:G:O2'   | 1:CA:1155:G:O5'    | 2.39                     | 0.40              |
| 1:CA:1168:A:H3'   | 1:CA:1169:A:C8     | 2.49                     | 0.40              |
| 1:CA:1168:A:C3'   | 1:CA:1169:A:H8     | 2.32                     | 0.40              |
| 1:CA:1188:A:H2'   | 1:CA:1189:C:H5'    | 2.02                     | 0.40              |
| 1:CA:134:A:N6     | 16:CP:25:ARG:NH1   | 2.66                     | 0.40              |
| 1:CA:1400:C:N4    | 24:CX:34:C:C6      | 2.89                     | 0.40              |
| 1:CA:275:G:H2'    | 1:CA:276:G:C8      | 2.56                     | 0.40              |
| 1:CA:321:A:C2     | 1:CA:333:G:C2      | 3.09                     | 0.40              |
| 1:CA:401:C:O2'    | 1:CA:402:G:H5'     | 2.22                     | 0.40              |
| 1:CA:509:A:N3     | 1:CA:543:C:O2'     | 2.43                     | 0.40              |
| 1:CA:528:C:O2'    | 1:CA:529:G:H5'     | 2.21                     | 0.40              |
| 1:CA:681:C:H2'    | 1:CA:682:G:C8      | 2.56                     | 0.40              |
| 1:CA:751:U:O4     | 1:CA:752:G:C2      | 2.74                     | 0.40              |
| 1:CA:929:G:H8     | 1:CA:929:G:O5'     | 2.05                     | 0.40              |
| 2:CB:134:GLU:HA   | 2:CB:137:ARG:HB2   | 2.04                     | 0.40              |
| 3:CC:14:ILE:O     | 3:CC:15:THR:C      | 2.60                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CC:39:ILE:HG22  | 3:CC:43:LEU:HD11   | 1.99                     | 0.40              |
| 3:CC:89:GLU:OE2   | 3:CC:89:GLU:O      | 2.39                     | 0.40              |
| 4:CD:77:ASN:O     | 4:CD:80:GLU:HB2    | 2.22                     | 0.40              |
| 5:CE:86:ALA:CB    | 5:CE:130:ASN:HD22  | 2.32                     | 0.40              |
| 5:CE:139:LEU:C    | 5:CE:141:GLN:H     | 2.24                     | 0.40              |
| 7:CG:144:MET:O    | 7:CG:147:ALA:HB3   | 2.21                     | 0.40              |
| 7:CG:155:ARG:O    | 7:CG:156:TRP:C     | 2.60                     | 0.40              |
| 8:CH:45:ILE:C     | 8:CH:47:GLY:N      | 2.74                     | 0.40              |
| 9:CI:65:VAL:CG1   | 9:CI:73:GLN:NE2    | 2.85                     | 0.40              |
| 9:CI:89:ASN:HA    | 9:CI:90:PRO:HD2    | 1.91                     | 0.40              |
| 13:CM:46:LYS:HG2  | 13:CM:47:ASP:OD1   | 2.20                     | 0.40              |
| 15:CO:41:GLU:O    | 15:CO:44:LYS:HB3   | 2.22                     | 0.40              |
| 16:CP:11:SER:HB2  | 16:CP:12:LYS:H     | 1.60                     | 0.40              |
| 24:CX:32:C:O2'    | 24:CX:33:U:H5'     | 2.22                     | 0.40              |
| 24:CX:47:U:H2'    | 24:CX:50:U:OP1     | 2.21                     | 0.40              |
| 49:D0:5:LYS:O     | 49:D0:6:GLY:C      | 2.60                     | 0.40              |
| 51:D2:41:ILE:HG13 | 51:D2:42:GLY:O     | 2.22                     | 0.40              |
| 51:D2:43:GLN:O    | 51:D2:44:LEU:CB    | 2.61                     | 0.40              |
| 52:D3:20:LYS:C    | 52:D3:22:ALA:H     | 2.24                     | 0.40              |
| 52:D3:40:THR:C    | 52:D3:42:ALA:N     | 2.74                     | 0.40              |
| 54:D5:46:CYS:HA   | 54:D5:47:PRO:HD2   | 1.93                     | 0.40              |
| 56:D7:16:HIS:O    | 56:D7:44:PRO:HD2   | 2.21                     | 0.40              |
| 27:DA:1041:C:H5'  | 27:DA:1042:G:OP2   | 2.22                     | 0.40              |
| 27:DA:1170:G:H1   | 27:DA:1179:C:N4    | 2.19                     | 0.40              |
| 27:DA:1444:G:H2'  | 27:DA:1445(A):C:C5 | 2.56                     | 0.40              |
| 27:DA:1629:U:O2'  | 27:DA:1630:G:H5'   | 2.21                     | 0.40              |
| 27:DA:1793:C:O2   | 27:DA:1970:A:C2    | 2.75                     | 0.40              |
| 27:DA:529:A:H62   | 27:DA:2041:U:H3    | 1.69                     | 0.40              |
| 27:DA:2158:A:H1'  | 27:DA:2159:G:C8    | 2.56                     | 0.40              |
| 27:DA:2163:C:OP1  | 27:DA:2165:G:O6    | 2.40                     | 0.40              |
| 27:DA:2182:G:C2   | 27:DA:2183:C:N3    | 2.89                     | 0.40              |
| 27:DA:219:G:H2'   | 27:DA:220:G:C8     | 2.56                     | 0.40              |
| 27:DA:2218:U:H3'  | 27:DA:2218:U:H6    | 1.87                     | 0.40              |
| 27:DA:2255:G:H2'  | 27:DA:2256:G:C8    | 2.57                     | 0.40              |
| 27:DA:2280:G:O2'  | 27:DA:2281:C:H5'   | 2.22                     | 0.40              |
| 27:DA:2348:U:OP2  | 57:D8:38:GLY:HA3   | 2.22                     | 0.40              |
| 27:DA:2369:A:H2'  | 27:DA:2370:G:H8    | 1.86                     | 0.40              |
| 27:DA:2393:A:H5'  | 38:DP:62:LEU:HB2   | 2.03                     | 0.40              |
| 27:DA:245:G:C5    | 27:DA:246:C:C5     | 3.09                     | 0.40              |
| 27:DA:2561:A:C4   | 27:DA:2562:U:C6    | 3.10                     | 0.40              |
| 27:DA:2600:A:C6   | 27:DA:2601:C:N4    | 2.90                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DA:2683:C:C6    | 27:DA:2684:U:C5   | 3.09                     | 0.40              |
| 27:DA:287:C:H6     | 27:DA:287:C:C5'   | 2.27                     | 0.40              |
| 27:DA:311:A:N9     | 27:DA:332:A:N7    | 2.70                     | 0.40              |
| 27:DA:460:A:H3'    | 27:DA:461:C:C6    | 2.56                     | 0.40              |
| 27:DA:500:G:N1     | 27:DA:503:A:OP2   | 2.54                     | 0.40              |
| 27:DA:68:G:H2'     | 27:DA:68:G:N3     | 2.36                     | 0.40              |
| 27:DA:831:G:H5'    | 27:DA:944:G:H22   | 1.87                     | 0.40              |
| 27:DA:960:A:C8     | 27:DA:962:G:C8    | 3.10                     | 0.40              |
| 28:DB:66:A:C2'     | 28:DB:67:G:OP2    | 2.69                     | 0.40              |
| 30:DD:29:PRO:O     | 30:DD:29:PRO:HG2  | 2.20                     | 0.40              |
| 30:DD:57:GLY:N     | 30:DD:216:GLY:HA2 | 2.36                     | 0.40              |
| 32:DF:107:LYS:HD3  | 32:DF:205:ARG:O   | 2.22                     | 0.40              |
| 32:DF:170:LEU:HD12 | 32:DF:170:LEU:HA  | 1.88                     | 0.40              |
| 33:DG:106:LEU:HA   | 33:DG:110:ALA:HB3 | 2.03                     | 0.40              |
| 33:DG:111:LEU:HD11 | 33:DG:120:LEU:CD2 | 2.39                     | 0.40              |
| 28:DB:45:A:O4'     | 33:DG:95:ARG:NH1  | 2.55                     | 0.40              |
| 35:DI:11:ASN:O     | 35:DI:12:LEU:HD22 | 2.20                     | 0.40              |
| 36:DN:86:PRO:HG2   | 36:DN:89:LYS:CB   | 2.50                     | 0.40              |
| 38:DP:61:ARG:HH11  | 57:D8:13:ARG:HD2  | 1.86                     | 0.40              |
| 27:DA:389:G:N1     | 38:DP:70:GLN:HG3  | 2.37                     | 0.40              |
| 45:DW:111:HIS:CG   | 45:DW:112:GLY:H   | 2.39                     | 0.40              |
| 45:DW:17:VAL:HG23  | 45:DW:18:ARG:N    | 2.37                     | 0.40              |
| 48:DZ:43:PHE:CZ    | 48:DZ:85:VAL:HG11 | 2.57                     | 0.40              |
| 48:DZ:78:ARG:O     | 48:DZ:79:ARG:HB2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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    | 233/256 (91%) | 126 (54%) | 73 (31%) | 34 (15%) | <b>0</b> <b>1</b> |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | CB    | 233/256 (91%) | 151 (65%) | 50 (22%) | 32 (14%) | 0           | 1  |
| 3   | AC    | 205/239 (86%) | 123 (60%) | 54 (26%) | 28 (14%) | 0           | 1  |
| 3   | CC    | 205/239 (86%) | 121 (59%) | 59 (29%) | 25 (12%) | 0           | 1  |
| 4   | AD    | 206/209 (99%) | 129 (63%) | 52 (25%) | 25 (12%) | 0           | 2  |
| 4   | CD    | 206/209 (99%) | 126 (61%) | 51 (25%) | 29 (14%) | 0           | 1  |
| 5   | AE    | 149/162 (92%) | 94 (63%)  | 38 (26%) | 17 (11%) | 0           | 2  |
| 5   | CE    | 149/162 (92%) | 103 (69%) | 27 (18%) | 19 (13%) | 0           | 1  |
| 6   | AF    | 99/101 (98%)  | 71 (72%)  | 18 (18%) | 10 (10%) | 1           | 3  |
| 6   | CF    | 99/101 (98%)  | 76 (77%)  | 16 (16%) | 7 (7%)   | 1           | 6  |
| 7   | AG    | 153/156 (98%) | 101 (66%) | 39 (26%) | 13 (8%)  | 1           | 4  |
| 7   | CG    | 153/156 (98%) | 102 (67%) | 38 (25%) | 13 (8%)  | 1           | 4  |
| 8   | AH    | 136/138 (99%) | 98 (72%)  | 27 (20%) | 11 (8%)  | 1           | 5  |
| 8   | CH    | 136/138 (99%) | 81 (60%)  | 38 (28%) | 17 (12%) | 0           | 1  |
| 9   | AI    | 125/128 (98%) | 83 (66%)  | 29 (23%) | 13 (10%) | 0           | 3  |
| 9   | CI    | 125/128 (98%) | 82 (66%)  | 26 (21%) | 17 (14%) | 0           | 1  |
| 10  | AJ    | 97/105 (92%)  | 64 (66%)  | 26 (27%) | 7 (7%)   | 1           | 6  |
| 10  | CJ    | 97/105 (92%)  | 55 (57%)  | 28 (29%) | 14 (14%) | 0           | 1  |
| 11  | AK    | 117/129 (91%) | 70 (60%)  | 34 (29%) | 13 (11%) | 0           | 2  |
| 11  | CK    | 117/129 (91%) | 87 (74%)  | 22 (19%) | 8 (7%)   | 1           | 7  |
| 12  | AL    | 123/132 (93%) | 75 (61%)  | 25 (20%) | 23 (19%) | 0           | 0  |
| 12  | CL    | 123/132 (93%) | 76 (62%)  | 24 (20%) | 23 (19%) | 0           | 0  |
| 13  | AM    | 118/126 (94%) | 64 (54%)  | 33 (28%) | 21 (18%) | 0           | 0  |
| 13  | CM    | 117/126 (93%) | 64 (55%)  | 29 (25%) | 24 (20%) | 0           | 0  |
| 14  | AN    | 58/61 (95%)   | 29 (50%)  | 19 (33%) | 10 (17%) | 0           | 1  |
| 14  | CN    | 58/61 (95%)   | 35 (60%)  | 12 (21%) | 11 (19%) | 0           | 0  |
| 15  | AO    | 86/89 (97%)   | 56 (65%)  | 19 (22%) | 11 (13%) | 0           | 1  |
| 15  | CO    | 86/89 (97%)   | 49 (57%)  | 28 (33%) | 9 (10%)  | 0           | 2  |
| 16  | AP    | 82/88 (93%)   | 49 (60%)  | 21 (26%) | 12 (15%) | 0           | 1  |
| 16  | CP    | 82/88 (93%)   | 45 (55%)  | 28 (34%) | 9 (11%)  | 0           | 2  |
| 17  | AQ    | 98/105 (93%)  | 73 (74%)  | 15 (15%) | 10 (10%) | 1           | 3  |
| 17  | CQ    | 98/105 (93%)  | 70 (71%)  | 22 (22%) | 6 (6%)   | 2           | 10 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 18  | AR    | 68/88 (77%)   | 35 (52%)  | 21 (31%) | 12 (18%) | 0           | 0   |
| 18  | CR    | 68/88 (77%)   | 41 (60%)  | 16 (24%) | 11 (16%) | 0           | 1   |
| 19  | AS    | 77/93 (83%)   | 51 (66%)  | 15 (20%) | 11 (14%) | 0           | 1   |
| 19  | CS    | 77/93 (83%)   | 46 (60%)  | 18 (23%) | 13 (17%) | 0           | 1   |
| 20  | AT    | 97/106 (92%)  | 59 (61%)  | 20 (21%) | 18 (19%) | 0           | 0   |
| 20  | CT    | 97/106 (92%)  | 52 (54%)  | 36 (37%) | 9 (9%)   | 1           | 4   |
| 21  | AU    | 23/27 (85%)   | 16 (70%)  | 4 (17%)  | 3 (13%)  | 0           | 1   |
| 21  | CU    | 23/27 (85%)   | 14 (61%)  | 5 (22%)  | 4 (17%)  | 0           | 1   |
| 26  | AZ    | 2/6 (33%)     | 1 (50%)   | 1 (50%)  | 0        | 100         | 100 |
| 26  | CZ    | 2/6 (33%)     | 1 (50%)   | 1 (50%)  | 0        | 100         | 100 |
| 29  | BC    | 183/229 (80%) | 69 (38%)  | 49 (27%) | 65 (36%) | 0           | 0   |
| 29  | DC    | 183/229 (80%) | 69 (38%)  | 59 (32%) | 55 (30%) | 0           | 0   |
| 30  | BD    | 270/276 (98%) | 172 (64%) | 66 (24%) | 32 (12%) | 0           | 2   |
| 30  | DD    | 270/276 (98%) | 180 (67%) | 57 (21%) | 33 (12%) | 0           | 1   |
| 31  | BE    | 203/206 (98%) | 130 (64%) | 38 (19%) | 35 (17%) | 0           | 1   |
| 31  | DE    | 203/206 (98%) | 125 (62%) | 34 (17%) | 44 (22%) | 0           | 0   |
| 32  | BF    | 206/210 (98%) | 137 (66%) | 31 (15%) | 38 (18%) | 0           | 0   |
| 32  | DF    | 206/210 (98%) | 125 (61%) | 40 (19%) | 41 (20%) | 0           | 0   |
| 33  | BG    | 179/182 (98%) | 107 (60%) | 47 (26%) | 25 (14%) | 0           | 1   |
| 33  | DG    | 179/182 (98%) | 109 (61%) | 42 (24%) | 28 (16%) | 0           | 1   |
| 34  | BH    | 162/180 (90%) | 87 (54%)  | 43 (26%) | 32 (20%) | 0           | 0   |
| 34  | DH    | 158/180 (88%) | 88 (56%)  | 35 (22%) | 35 (22%) | 0           | 0   |
| 35  | BI    | 144/148 (97%) | 73 (51%)  | 33 (23%) | 38 (26%) | 0           | 0   |
| 35  | DI    | 144/148 (97%) | 80 (56%)  | 41 (28%) | 23 (16%) | 0           | 1   |
| 36  | BN    | 137/140 (98%) | 91 (66%)  | 27 (20%) | 19 (14%) | 0           | 1   |
| 36  | DN    | 137/140 (98%) | 82 (60%)  | 28 (20%) | 27 (20%) | 0           | 0   |
| 37  | BO    | 120/122 (98%) | 84 (70%)  | 25 (21%) | 11 (9%)  | 1           | 4   |
| 37  | DO    | 120/122 (98%) | 80 (67%)  | 23 (19%) | 17 (14%) | 0           | 1   |
| 38  | BP    | 144/150 (96%) | 71 (49%)  | 42 (29%) | 31 (22%) | 0           | 0   |
| 38  | DP    | 144/150 (96%) | 72 (50%)  | 36 (25%) | 36 (25%) | 0           | 0   |
| 39  | BQ    | 139/141 (99%) | 98 (70%)  | 21 (15%) | 20 (14%) | 0           | 1   |

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| Mol | Chain | Analysed      | Favoured | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|----------|----------|----------|-------------|----|
| 39  | DQ    | 137/141 (97%) | 88 (64%) | 29 (21%) | 20 (15%) | 0           | 1  |
| 40  | BR    | 115/118 (98%) | 75 (65%) | 25 (22%) | 15 (13%) | 0           | 1  |
| 40  | DR    | 115/118 (98%) | 66 (57%) | 31 (27%) | 18 (16%) | 0           | 1  |
| 41  | BS    | 97/112 (87%)  | 45 (46%) | 24 (25%) | 28 (29%) | 0           | 0  |
| 41  | DS    | 99/112 (88%)  | 51 (52%) | 14 (14%) | 34 (34%) | 0           | 0  |
| 42  | BT    | 136/146 (93%) | 78 (57%) | 26 (19%) | 32 (24%) | 0           | 0  |
| 42  | DT    | 136/146 (93%) | 68 (50%) | 32 (24%) | 36 (26%) | 0           | 0  |
| 43  | BU    | 115/118 (98%) | 70 (61%) | 27 (24%) | 18 (16%) | 0           | 1  |
| 43  | DU    | 115/118 (98%) | 69 (60%) | 30 (26%) | 16 (14%) | 0           | 1  |
| 44  | BV    | 99/101 (98%)  | 61 (62%) | 24 (24%) | 14 (14%) | 0           | 1  |
| 44  | DV    | 99/101 (98%)  | 61 (62%) | 19 (19%) | 19 (19%) | 0           | 0  |
| 45  | BW    | 111/113 (98%) | 77 (69%) | 23 (21%) | 11 (10%) | 1           | 3  |
| 45  | DW    | 111/113 (98%) | 71 (64%) | 29 (26%) | 11 (10%) | 1           | 3  |
| 46  | BX    | 91/96 (95%)   | 67 (74%) | 16 (18%) | 8 (9%)   | 1           | 4  |
| 46  | DX    | 91/96 (95%)   | 60 (66%) | 17 (19%) | 14 (15%) | 0           | 1  |
| 47  | BY    | 99/110 (90%)  | 42 (42%) | 22 (22%) | 35 (35%) | 0           | 0  |
| 47  | DY    | 99/110 (90%)  | 37 (37%) | 29 (29%) | 33 (33%) | 0           | 0  |
| 48  | BZ    | 175/206 (85%) | 99 (57%) | 49 (28%) | 27 (15%) | 0           | 1  |
| 48  | DZ    | 175/206 (85%) | 97 (55%) | 51 (29%) | 27 (15%) | 0           | 1  |
| 49  | B0    | 82/85 (96%)   | 62 (76%) | 12 (15%) | 8 (10%)  | 1           | 3  |
| 49  | D0    | 82/85 (96%)   | 61 (74%) | 14 (17%) | 7 (8%)   | 1           | 4  |
| 50  | B1    | 92/98 (94%)   | 60 (65%) | 20 (22%) | 12 (13%) | 0           | 1  |
| 50  | D1    | 92/98 (94%)   | 65 (71%) | 16 (17%) | 11 (12%) | 0           | 2  |
| 51  | B2    | 69/72 (96%)   | 46 (67%) | 14 (20%) | 9 (13%)  | 0           | 1  |
| 51  | D2    | 69/72 (96%)   | 37 (54%) | 20 (29%) | 12 (17%) | 0           | 1  |
| 52  | B3    | 58/60 (97%)   | 49 (84%) | 7 (12%)  | 2 (3%)   | 4           | 24 |
| 52  | D3    | 58/60 (97%)   | 46 (79%) | 10 (17%) | 2 (3%)   | 4           | 24 |
| 53  | B4    | 29/71 (41%)   | 18 (62%) | 6 (21%)  | 5 (17%)  | 0           | 1  |
| 53  | D4    | 29/71 (41%)   | 17 (59%) | 9 (31%)  | 3 (10%)  | 0           | 3  |
| 54  | B5    | 57/60 (95%)   | 34 (60%) | 13 (23%) | 10 (18%) | 0           | 1  |
| 54  | D5    | 57/60 (95%)   | 33 (58%) | 14 (25%) | 10 (18%) | 0           | 1  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 55  | B6    | 49/54 (91%)       | 17 (35%)   | 14 (29%)   | 18 (37%)   | 0           | 0  |
| 55  | D6    | 44/54 (82%)       | 16 (36%)   | 11 (25%)   | 17 (39%)   | 0           | 0  |
| 56  | B7    | 47/49 (96%)       | 35 (74%)   | 8 (17%)    | 4 (8%)     | 1           | 4  |
| 56  | D7    | 47/49 (96%)       | 30 (64%)   | 13 (28%)   | 4 (8%)     | 1           | 4  |
| 57  | B8    | 62/65 (95%)       | 34 (55%)   | 19 (31%)   | 9 (14%)    | 0           | 1  |
| 57  | D8    | 62/65 (95%)       | 32 (52%)   | 15 (24%)   | 15 (24%)   | 0           | 0  |
| 58  | B9    | 34/37 (92%)       | 25 (74%)   | 8 (24%)    | 1 (3%)     | 5           | 28 |
| 58  | D9    | 34/37 (92%)       | 18 (53%)   | 13 (38%)   | 3 (9%)     | 1           | 4  |
| All | All   | 11702/12598 (93%) | 7090 (61%) | 2747 (24%) | 1865 (16%) | 0           | 1  |

All (1865) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 9   | GLU  |
| 2   | AB    | 15  | VAL  |
| 2   | AB    | 20  | GLU  |
| 2   | AB    | 96  | ARG  |
| 2   | AB    | 101 | MET  |
| 2   | AB    | 194 | PRO  |
| 2   | AB    | 229 | VAL  |
| 3   | AC    | 51  | GLY  |
| 3   | AC    | 61  | ALA  |
| 3   | AC    | 101 | LEU  |
| 3   | AC    | 113 | ALA  |
| 3   | AC    | 127 | ARG  |
| 3   | AC    | 135 | LYS  |
| 3   | AC    | 165 | THR  |
| 4   | AD    | 146 | ILE  |
| 4   | AD    | 179 | GLU  |
| 5   | AE    | 21  | ALA  |
| 5   | AE    | 129 | ILE  |
| 5   | AE    | 130 | ASN  |
| 5   | AE    | 141 | GLN  |
| 6   | AF    | 13  | ASN  |
| 6   | AF    | 16  | GLN  |
| 6   | AF    | 62  | TRP  |
| 7   | AG    | 7   | ALA  |
| 7   | AG    | 52  | GLU  |
| 7   | AG    | 53  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | AG    | 58  | PRO  |
| 7   | AG    | 155 | ARG  |
| 8   | AH    | 6   | ILE  |
| 8   | AH    | 49  | GLU  |
| 8   | AH    | 77  | GLU  |
| 8   | AH    | 91  | ARG  |
| 8   | AH    | 97  | VAL  |
| 9   | AI    | 12  | GLU  |
| 9   | AI    | 23  | ASN  |
| 9   | AI    | 54  | ASP  |
| 9   | AI    | 61  | ALA  |
| 9   | AI    | 107 | ARG  |
| 10  | AJ    | 32  | ALA  |
| 11  | AK    | 24  | SER  |
| 11  | AK    | 48  | ILE  |
| 11  | AK    | 77  | MET  |
| 11  | AK    | 86  | GLY  |
| 11  | AK    | 89  | ALA  |
| 12  | AL    | 38  | ARG  |
| 12  | AL    | 44  | LYS  |
| 12  | AL    | 74  | LEU  |
| 12  | AL    | 86  | ARG  |
| 12  | AL    | 125 | ALA  |
| 13  | AM    | 12  | ASN  |
| 13  | AM    | 95  | GLY  |
| 13  | AM    | 117 | VAL  |
| 14  | AN    | 14  | PRO  |
| 14  | AN    | 15  | LYS  |
| 14  | AN    | 16  | PHE  |
| 14  | AN    | 28  | GLY  |
| 14  | AN    | 52  | GLN  |
| 14  | AN    | 59  | ALA  |
| 15  | AO    | 29  | VAL  |
| 16  | AP    | 24  | ALA  |
| 16  | AP    | 25  | ARG  |
| 16  | AP    | 45  | THR  |
| 17  | AQ    | 33  | GLY  |
| 18  | AR    | 20  | ALA  |
| 18  | AR    | 37  | VAL  |
| 18  | AR    | 87  | ARG  |
| 19  | AS    | 6   | LYS  |
| 19  | AS    | 10  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | AS    | 25  | LYS  |
| 19  | AS    | 28  | LYS  |
| 19  | AS    | 30  | LEU  |
| 19  | AS    | 61  | TYR  |
| 19  | AS    | 62  | ILE  |
| 19  | AS    | 80  | TYR  |
| 20  | AT    | 28  | ALA  |
| 20  | AT    | 49  | ALA  |
| 20  | AT    | 63  | ILE  |
| 20  | AT    | 74  | LYS  |
| 29  | BC    | 38  | ASP  |
| 29  | BC    | 46  | LYS  |
| 29  | BC    | 52  | ARG  |
| 29  | BC    | 55  | ASP  |
| 29  | BC    | 140 | PRO  |
| 29  | BC    | 142 | ALA  |
| 29  | BC    | 148 | ASN  |
| 29  | BC    | 153 | ILE  |
| 29  | BC    | 156 | ILE  |
| 29  | BC    | 162 | GLU  |
| 29  | BC    | 166 | ASP  |
| 29  | BC    | 167 | LYS  |
| 29  | BC    | 170 | ALA  |
| 29  | BC    | 173 | ALA  |
| 29  | BC    | 174 | PRO  |
| 29  | BC    | 182 | PRO  |
| 29  | BC    | 193 | ILE  |
| 29  | BC    | 194 | ARG  |
| 29  | BC    | 195 | ALA  |
| 29  | BC    | 211 | SER  |
| 29  | BC    | 216 | THR  |
| 29  | BC    | 220 | PRO  |
| 29  | BC    | 222 | VAL  |
| 30  | BD    | 3   | VAL  |
| 30  | BD    | 25  | THR  |
| 30  | BD    | 33  | LEU  |
| 30  | BD    | 118 | VAL  |
| 30  | BD    | 169 | GLU  |
| 30  | BD    | 198 | ASN  |
| 30  | BD    | 211 | ARG  |
| 30  | BD    | 242 | ARG  |
| 30  | BD    | 268 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BD    | 271 | ILE  |
| 31  | BE    | 4   | ILE  |
| 31  | BE    | 18  | ASP  |
| 31  | BE    | 46  | ALA  |
| 31  | BE    | 53  | PRO  |
| 31  | BE    | 54  | GLN  |
| 31  | BE    | 55  | ASN  |
| 31  | BE    | 72  | VAL  |
| 31  | BE    | 75  | VAL  |
| 31  | BE    | 77  | ILE  |
| 31  | BE    | 82  | ARG  |
| 31  | BE    | 94  | GLU  |
| 31  | BE    | 118 | LYS  |
| 31  | BE    | 129 | HIS  |
| 31  | BE    | 131 | ALA  |
| 31  | BE    | 174 | ASP  |
| 31  | BE    | 187 | ALA  |
| 31  | BE    | 200 | GLU  |
| 32  | BF    | 4   | VAL  |
| 32  | BF    | 5   | ALA  |
| 32  | BF    | 22  | ALA  |
| 32  | BF    | 25  | PRO  |
| 32  | BF    | 62  | ARG  |
| 32  | BF    | 65  | TRP  |
| 32  | BF    | 68  | LYS  |
| 32  | BF    | 69  | HIS  |
| 32  | BF    | 74  | ARG  |
| 32  | BF    | 84  | VAL  |
| 32  | BF    | 90  | PHE  |
| 32  | BF    | 123 | LEU  |
| 32  | BF    | 127 | GLU  |
| 32  | BF    | 132 | VAL  |
| 32  | BF    | 160 | ASN  |
| 33  | BG    | 27  | ASN  |
| 33  | BG    | 47  | LYS  |
| 33  | BG    | 81  | LYS  |
| 33  | BG    | 82  | LEU  |
| 33  | BG    | 87  | PRO  |
| 33  | BG    | 96  | ARG  |
| 33  | BG    | 97  | ASP  |
| 33  | BG    | 115 | ARG  |
| 33  | BG    | 124 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | BG    | 126 | ASP  |
| 33  | BG    | 179 | PRO  |
| 34  | BH    | 9   | ILE  |
| 34  | BH    | 10  | PRO  |
| 34  | BH    | 12  | PRO  |
| 34  | BH    | 13  | LYS  |
| 34  | BH    | 21  | PRO  |
| 34  | BH    | 45  | VAL  |
| 34  | BH    | 54  | ARG  |
| 34  | BH    | 71  | LEU  |
| 34  | BH    | 83  | TYR  |
| 34  | BH    | 90  | LYS  |
| 34  | BH    | 92  | ILE  |
| 34  | BH    | 99  | VAL  |
| 34  | BH    | 108 | GLY  |
| 34  | BH    | 127 | GLU  |
| 34  | BH    | 138 | LYS  |
| 34  | BH    | 155 | SER  |
| 34  | BH    | 156 | ALA  |
| 34  | BH    | 158 | HIS  |
| 34  | BH    | 159 | GLU  |
| 34  | BH    | 165 | ALA  |
| 34  | BH    | 169 | VAL  |
| 34  | BH    | 170 | ARG  |
| 35  | BI    | 42  | SER  |
| 35  | BI    | 68  | LEU  |
| 35  | BI    | 83  | ALA  |
| 35  | BI    | 87  | LYS  |
| 35  | BI    | 91  | SER  |
| 35  | BI    | 92  | VAL  |
| 35  | BI    | 120 | ILE  |
| 36  | BN    | 47  | ALA  |
| 36  | BN    | 58  | ASP  |
| 36  | BN    | 68  | GLU  |
| 36  | BN    | 77  | GLY  |
| 36  | BN    | 94  | HIS  |
| 36  | BN    | 120 | LEU  |
| 37  | BO    | 58  | VAL  |
| 37  | BO    | 98  | VAL  |
| 37  | BO    | 109 | LYS  |
| 38  | BP    | 9   | ASN  |
| 38  | BP    | 11  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BP    | 14  | LYS  |
| 38  | BP    | 25  | SER  |
| 38  | BP    | 31  | ALA  |
| 38  | BP    | 47  | ASP  |
| 38  | BP    | 89  | ALA  |
| 38  | BP    | 106 | LEU  |
| 38  | BP    | 108 | LYS  |
| 39  | BQ    | 6   | ARG  |
| 39  | BQ    | 19  | GLY  |
| 39  | BQ    | 20  | ALA  |
| 39  | BQ    | 47  | ILE  |
| 39  | BQ    | 57  | HIS  |
| 39  | BQ    | 63  | LYS  |
| 39  | BQ    | 115 | MET  |
| 39  | BQ    | 134 | ARG  |
| 39  | BQ    | 136 | ALA  |
| 40  | BR    | 8   | ARG  |
| 40  | BR    | 14  | SER  |
| 40  | BR    | 102 | GLU  |
| 41  | BS    | 18  | ILE  |
| 41  | BS    | 23  | ARG  |
| 41  | BS    | 35  | ILE  |
| 41  | BS    | 53  | SER  |
| 41  | BS    | 58  | LEU  |
| 41  | BS    | 62  | LYS  |
| 41  | BS    | 78  | LEU  |
| 41  | BS    | 82  | ILE  |
| 41  | BS    | 88  | ASP  |
| 41  | BS    | 94  | TYR  |
| 41  | BS    | 96  | GLY  |
| 41  | BS    | 102 | ALA  |
| 42  | BT    | 14  | TYR  |
| 42  | BT    | 27  | THR  |
| 42  | BT    | 28  | VAL  |
| 42  | BT    | 30  | VAL  |
| 42  | BT    | 33  | LYS  |
| 42  | BT    | 35  | LYS  |
| 42  | BT    | 39  | ARG  |
| 42  | BT    | 41  | ARG  |
| 42  | BT    | 55  | ASN  |
| 42  | BT    | 69  | GLY  |
| 42  | BT    | 80  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | BT    | 81  | PRO  |
| 42  | BT    | 83  | ILE  |
| 42  | BT    | 94  | ALA  |
| 42  | BT    | 107 | ASP  |
| 42  | BT    | 116 | ALA  |
| 43  | BU    | 9   | VAL  |
| 43  | BU    | 26  | GLY  |
| 43  | BU    | 32  | PHE  |
| 43  | BU    | 42  | ALA  |
| 43  | BU    | 43  | GLY  |
| 43  | BU    | 74  | LEU  |
| 43  | BU    | 76  | TYR  |
| 43  | BU    | 90  | VAL  |
| 43  | BU    | 91  | ASP  |
| 43  | BU    | 93  | LYS  |
| 44  | BV    | 3   | ALA  |
| 44  | BV    | 16  | PRO  |
| 44  | BV    | 19  | LYS  |
| 44  | BV    | 29  | PRO  |
| 44  | BV    | 46  | VAL  |
| 44  | BV    | 49  | THR  |
| 44  | BV    | 50  | PRO  |
| 45  | BW    | 14  | PRO  |
| 45  | BW    | 44  | ALA  |
| 45  | BW    | 65  | LEU  |
| 46  | BX    | 12  | VAL  |
| 46  | BX    | 34  | ALA  |
| 46  | BX    | 93  | GLU  |
| 47  | BY    | 3   | VAL  |
| 47  | BY    | 5   | MET  |
| 47  | BY    | 31  | LEU  |
| 47  | BY    | 38  | ILE  |
| 47  | BY    | 40  | GLU  |
| 47  | BY    | 48  | ALA  |
| 47  | BY    | 50  | ARG  |
| 47  | BY    | 52  | SER  |
| 47  | BY    | 53  | PRO  |
| 47  | BY    | 56  | PRO  |
| 47  | BY    | 62  | GLU  |
| 47  | BY    | 64  | GLU  |
| 47  | BY    | 66  | PRO  |
| 47  | BY    | 68  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | BY    | 75  | ILE  |
| 47  | BY    | 77  | PRO  |
| 47  | BY    | 78  | ALA  |
| 47  | BY    | 87  | LYS  |
| 47  | BY    | 88  | LYS  |
| 47  | BY    | 98  | VAL  |
| 48  | BZ    | 29  | ASN  |
| 48  | BZ    | 34  | ARG  |
| 48  | BZ    | 64  | GLN  |
| 48  | BZ    | 80  | ARG  |
| 48  | BZ    | 104 | VAL  |
| 48  | BZ    | 120 | HIS  |
| 48  | BZ    | 145 | ILE  |
| 48  | BZ    | 150 | HIS  |
| 48  | BZ    | 151 | ALA  |
| 48  | BZ    | 167 | GLU  |
| 49  | B0    | 18  | ALA  |
| 49  | B0    | 55  | ARG  |
| 50  | B1    | 4   | VAL  |
| 50  | B1    | 30  | VAL  |
| 50  | B1    | 38  | SER  |
| 50  | B1    | 52  | ARG  |
| 50  | B1    | 53  | VAL  |
| 50  | B1    | 76  | ARG  |
| 51  | B2    | 43  | GLN  |
| 51  | B2    | 47  | ASN  |
| 52  | B3    | 2   | PRO  |
| 53  | B4    | 61  | VAL  |
| 54  | B5    | 4   | HIS  |
| 54  | B5    | 32  | PRO  |
| 54  | B5    | 33  | CYS  |
| 54  | B5    | 35  | GLU  |
| 55  | B6    | 5   | VAL  |
| 55  | B6    | 7   | ILE  |
| 55  | B6    | 16  | CYS  |
| 55  | B6    | 17  | LYS  |
| 55  | B6    | 20  | ASN  |
| 55  | B6    | 29  | ASN  |
| 55  | B6    | 34  | LEU  |
| 55  | B6    | 46  | HIS  |
| 55  | B6    | 48  | VAL  |
| 55  | B6    | 52  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | B8    | 18  | ALA  |
| 57  | B8    | 34  | TRP  |
| 57  | B8    | 61  | LEU  |
| 58  | B9    | 15  | LYS  |
| 2   | CB    | 9   | GLU  |
| 2   | CB    | 15  | VAL  |
| 2   | CB    | 77  | ALA  |
| 2   | CB    | 159 | PRO  |
| 2   | CB    | 189 | ASP  |
| 2   | CB    | 194 | PRO  |
| 2   | CB    | 195 | ASP  |
| 2   | CB    | 208 | ILE  |
| 3   | CC    | 7   | PRO  |
| 3   | CC    | 12  | LEU  |
| 3   | CC    | 15  | THR  |
| 3   | CC    | 60  | ALA  |
| 3   | CC    | 134 | ILE  |
| 3   | CC    | 154 | SER  |
| 3   | CC    | 156 | ARG  |
| 3   | CC    | 180 | ALA  |
| 3   | CC    | 207 | VAL  |
| 4   | CD    | 14  | ARG  |
| 4   | CD    | 30  | LYS  |
| 4   | CD    | 39  | PRO  |
| 4   | CD    | 101 | LEU  |
| 5   | CE    | 7   | GLU  |
| 5   | CE    | 21  | ALA  |
| 5   | CE    | 129 | ILE  |
| 5   | CE    | 144 | THR  |
| 5   | CE    | 146 | ALA  |
| 5   | CE    | 147 | ASP  |
| 6   | CF    | 39  | LYS  |
| 6   | CF    | 44  | GLY  |
| 6   | CF    | 45  | LEU  |
| 7   | CG    | 15  | ASP  |
| 7   | CG    | 58  | PRO  |
| 7   | CG    | 77  | SER  |
| 7   | CG    | 78  | ARG  |
| 7   | CG    | 84  | ASN  |
| 8   | CH    | 2   | LEU  |
| 8   | CH    | 22  | GLU  |
| 8   | CH    | 83  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | CH    | 91  | ARG  |
| 9   | CI    | 54  | ASP  |
| 9   | CI    | 107 | ARG  |
| 10  | CJ    | 32  | ALA  |
| 10  | CJ    | 36  | GLY  |
| 10  | CJ    | 57  | LYS  |
| 10  | CJ    | 82  | ILE  |
| 10  | CJ    | 92  | THR  |
| 11  | CK    | 87  | THR  |
| 12  | CL    | 4   | ILE  |
| 12  | CL    | 15  | VAL  |
| 12  | CL    | 44  | LYS  |
| 12  | CL    | 61  | TYR  |
| 12  | CL    | 74  | LEU  |
| 12  | CL    | 112 | LYS  |
| 12  | CL    | 113 | SER  |
| 13  | CM    | 7   | VAL  |
| 13  | CM    | 48  | LEU  |
| 13  | CM    | 60  | VAL  |
| 13  | CM    | 67  | GLU  |
| 13  | CM    | 83  | ASP  |
| 13  | CM    | 95  | GLY  |
| 13  | CM    | 96  | LEU  |
| 13  | CM    | 113 | PRO  |
| 14  | CN    | 14  | PRO  |
| 14  | CN    | 16  | PHE  |
| 14  | CN    | 24  | CYS  |
| 15  | CO    | 13  | GLN  |
| 16  | CP    | 16  | HIS  |
| 16  | CP    | 77  | ALA  |
| 17  | CQ    | 34  | LYS  |
| 17  | CQ    | 78  | GLU  |
| 18  | CR    | 20  | ALA  |
| 18  | CR    | 54  | ARG  |
| 18  | CR    | 64  | ARG  |
| 18  | CR    | 65  | ILE  |
| 18  | CR    | 83  | GLU  |
| 18  | CR    | 87  | ARG  |
| 19  | CS    | 10  | PHE  |
| 19  | CS    | 25  | LYS  |
| 19  | CS    | 28  | LYS  |
| 19  | CS    | 31  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | CS    | 61  | TYR  |
| 19  | CS    | 62  | ILE  |
| 20  | CT    | 48  | LYS  |
| 20  | CT    | 49  | ALA  |
| 20  | CT    | 71  | THR  |
| 20  | CT    | 97  | ALA  |
| 21  | CU    | 9   | ARG  |
| 21  | CU    | 22  | ARG  |
| 21  | CU    | 25  | LYS  |
| 29  | DC    | 38  | ASP  |
| 29  | DC    | 46  | LYS  |
| 29  | DC    | 49  | ILE  |
| 29  | DC    | 63  | SER  |
| 29  | DC    | 108 | MET  |
| 29  | DC    | 122 | ALA  |
| 29  | DC    | 133 | PRO  |
| 29  | DC    | 148 | ASN  |
| 29  | DC    | 151 | GLU  |
| 29  | DC    | 153 | ILE  |
| 29  | DC    | 156 | ILE  |
| 29  | DC    | 166 | ASP  |
| 29  | DC    | 167 | LYS  |
| 29  | DC    | 173 | ALA  |
| 29  | DC    | 174 | PRO  |
| 29  | DC    | 182 | PRO  |
| 29  | DC    | 183 | GLU  |
| 29  | DC    | 209 | LEU  |
| 29  | DC    | 211 | SER  |
| 29  | DC    | 217 | THR  |
| 29  | DC    | 220 | PRO  |
| 29  | DC    | 222 | VAL  |
| 30  | DD    | 12  | SER  |
| 30  | DD    | 24  | ILE  |
| 30  | DD    | 27  | THR  |
| 30  | DD    | 33  | LEU  |
| 30  | DD    | 45  | ASN  |
| 30  | DD    | 76  | PRO  |
| 30  | DD    | 118 | VAL  |
| 30  | DD    | 224 | ALA  |
| 30  | DD    | 242 | ARG  |
| 30  | DD    | 245 | PRO  |
| 30  | DD    | 246 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DD    | 271 | ILE  |
| 31  | DE    | 4   | ILE  |
| 31  | DE    | 18  | ASP  |
| 31  | DE    | 20  | ALA  |
| 31  | DE    | 30  | PRO  |
| 31  | DE    | 35  | GLN  |
| 31  | DE    | 45  | THR  |
| 31  | DE    | 54  | GLN  |
| 31  | DE    | 55  | ASN  |
| 31  | DE    | 59  | VAL  |
| 31  | DE    | 60  | ASN  |
| 31  | DE    | 71  | GLY  |
| 31  | DE    | 75  | VAL  |
| 31  | DE    | 77  | ILE  |
| 31  | DE    | 117 | MET  |
| 31  | DE    | 131 | ALA  |
| 31  | DE    | 174 | ASP  |
| 31  | DE    | 185 | LYS  |
| 32  | DF    | 4   | VAL  |
| 32  | DF    | 8   | GLN  |
| 32  | DF    | 11  | VAL  |
| 32  | DF    | 25  | PRO  |
| 32  | DF    | 59  | TYR  |
| 32  | DF    | 62  | ARG  |
| 32  | DF    | 64  | ILE  |
| 32  | DF    | 66  | PRO  |
| 32  | DF    | 67  | GLN  |
| 32  | DF    | 68  | LYS  |
| 32  | DF    | 89  | VAL  |
| 32  | DF    | 116 | ASP  |
| 32  | DF    | 129 | PHE  |
| 32  | DF    | 132 | VAL  |
| 32  | DF    | 133 | ASN  |
| 32  | DF    | 168 | ARG  |
| 32  | DF    | 202 | PHE  |
| 32  | DF    | 203 | GLN  |
| 33  | DG    | 34  | LEU  |
| 33  | DG    | 47  | LYS  |
| 33  | DG    | 51  | ARG  |
| 33  | DG    | 52  | ILE  |
| 33  | DG    | 82  | LEU  |
| 33  | DG    | 87  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | DG    | 96  | ARG  |
| 33  | DG    | 97  | ASP  |
| 33  | DG    | 117 | PHE  |
| 33  | DG    | 126 | ASP  |
| 33  | DG    | 142 | PRO  |
| 34  | DH    | 24  | VAL  |
| 34  | DH    | 54  | ARG  |
| 34  | DH    | 55  | PRO  |
| 34  | DH    | 71  | LEU  |
| 34  | DH    | 83  | TYR  |
| 34  | DH    | 90  | LYS  |
| 34  | DH    | 92  | ILE  |
| 34  | DH    | 93  | GLY  |
| 34  | DH    | 109 | PHE  |
| 34  | DH    | 127 | GLU  |
| 34  | DH    | 155 | SER  |
| 34  | DH    | 156 | ALA  |
| 34  | DH    | 159 | GLU  |
| 34  | DH    | 160 | LYS  |
| 35  | DI    | 12  | LEU  |
| 35  | DI    | 40  | THR  |
| 35  | DI    | 42  | SER  |
| 35  | DI    | 77  | LEU  |
| 35  | DI    | 101 | LEU  |
| 35  | DI    | 117 | GLU  |
| 35  | DI    | 120 | ILE  |
| 35  | DI    | 130 | TYR  |
| 35  | DI    | 132 | PRO  |
| 36  | DN    | 4   | TYR  |
| 36  | DN    | 37  | LYS  |
| 36  | DN    | 42  | TRP  |
| 36  | DN    | 57  | ALA  |
| 36  | DN    | 59  | LYS  |
| 36  | DN    | 60  | ILE  |
| 36  | DN    | 77  | GLY  |
| 36  | DN    | 129 | PRO  |
| 37  | DO    | 6   | THR  |
| 37  | DO    | 48  | PRO  |
| 37  | DO    | 54  | GLU  |
| 37  | DO    | 101 | PRO  |
| 38  | DP    | 9   | ASN  |
| 38  | DP    | 11  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | DP    | 17  | LYS  |
| 38  | DP    | 19  | VAL  |
| 38  | DP    | 31  | ALA  |
| 38  | DP    | 33  | ARG  |
| 38  | DP    | 35  | HIS  |
| 38  | DP    | 47  | ASP  |
| 38  | DP    | 65  | ARG  |
| 38  | DP    | 69  | GLY  |
| 38  | DP    | 106 | LEU  |
| 38  | DP    | 107 | LYS  |
| 38  | DP    | 108 | LYS  |
| 38  | DP    | 122 | PRO  |
| 39  | DQ    | 2   | LEU  |
| 39  | DQ    | 5   | ARG  |
| 39  | DQ    | 62  | GLY  |
| 39  | DQ    | 83  | MET  |
| 39  | DQ    | 109 | VAL  |
| 39  | DQ    | 138 | ASP  |
| 40  | DR    | 9   | LYS  |
| 40  | DR    | 15  | SER  |
| 40  | DR    | 20  | LEU  |
| 40  | DR    | 45  | ARG  |
| 40  | DR    | 58  | GLY  |
| 40  | DR    | 102 | GLU  |
| 41  | DS    | 10  | ARG  |
| 41  | DS    | 11  | LYS  |
| 41  | DS    | 15  | ARG  |
| 41  | DS    | 19  | LYS  |
| 41  | DS    | 23  | ARG  |
| 41  | DS    | 32  | LEU  |
| 41  | DS    | 35  | ILE  |
| 41  | DS    | 44  | LYS  |
| 41  | DS    | 57  | LYS  |
| 41  | DS    | 58  | LEU  |
| 41  | DS    | 59  | LYS  |
| 41  | DS    | 62  | LYS  |
| 41  | DS    | 83  | LYS  |
| 41  | DS    | 92  | TYR  |
| 41  | DS    | 97  | ARG  |
| 41  | DS    | 100 | ALA  |
| 41  | DS    | 103 | GLU  |
| 42  | DT    | 17  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DT    | 24  | PRO  |
| 42  | DT    | 28  | VAL  |
| 42  | DT    | 30  | VAL  |
| 42  | DT    | 36  | GLU  |
| 42  | DT    | 39  | ARG  |
| 42  | DT    | 40  | THR  |
| 42  | DT    | 55  | ASN  |
| 42  | DT    | 81  | PRO  |
| 42  | DT    | 82  | LEU  |
| 42  | DT    | 83  | ILE  |
| 42  | DT    | 115 | ARG  |
| 42  | DT    | 136 | GLN  |
| 43  | DU    | 25  | TRP  |
| 43  | DU    | 79  | PHE  |
| 43  | DU    | 100 | VAL  |
| 44  | DV    | 3   | ALA  |
| 44  | DV    | 18  | LEU  |
| 44  | DV    | 29  | PRO  |
| 44  | DV    | 46  | VAL  |
| 44  | DV    | 77  | ALA  |
| 44  | DV    | 78  | LYS  |
| 44  | DV    | 79  | VAL  |
| 46  | DX    | 12  | VAL  |
| 46  | DX    | 44  | GLU  |
| 46  | DX    | 45  | THR  |
| 46  | DX    | 57  | LEU  |
| 46  | DX    | 91  | ALA  |
| 46  | DX    | 93  | GLU  |
| 47  | DY    | 3   | VAL  |
| 47  | DY    | 5   | MET  |
| 47  | DY    | 30  | VAL  |
| 47  | DY    | 44  | ILE  |
| 47  | DY    | 53  | PRO  |
| 47  | DY    | 56  | PRO  |
| 47  | DY    | 68  | HIS  |
| 47  | DY    | 77  | PRO  |
| 47  | DY    | 78  | ALA  |
| 47  | DY    | 82  | PRO  |
| 47  | DY    | 90  | LEU  |
| 47  | DY    | 101 | LYS  |
| 48  | DZ    | 29  | ASN  |
| 48  | DZ    | 30  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | DZ    | 48  | ARG  |
| 48  | DZ    | 64  | GLN  |
| 48  | DZ    | 80  | ARG  |
| 48  | DZ    | 95  | VAL  |
| 48  | DZ    | 104 | VAL  |
| 48  | DZ    | 110 | VAL  |
| 48  | DZ    | 144 | GLU  |
| 48  | DZ    | 157 | PRO  |
| 48  | DZ    | 171 | ALA  |
| 50  | D1    | 31  | GLY  |
| 50  | D1    | 58  | ILE  |
| 51  | D2    | 44  | LEU  |
| 51  | D2    | 47  | ASN  |
| 51  | D2    | 48  | HIS  |
| 51  | D2    | 70  | GLN  |
| 52  | D3    | 2   | PRO  |
| 53  | D4    | 52  | SER  |
| 54  | D5    | 4   | HIS  |
| 54  | D5    | 12  | SER  |
| 54  | D5    | 38  | ALA  |
| 54  | D5    | 57  | VAL  |
| 55  | D6    | 9   | LEU  |
| 55  | D6    | 16  | CYS  |
| 55  | D6    | 17  | LYS  |
| 55  | D6    | 20  | ASN  |
| 55  | D6    | 23  | THR  |
| 55  | D6    | 29  | ASN  |
| 55  | D6    | 46  | HIS  |
| 55  | D6    | 52  | VAL  |
| 56  | D7    | 13  | ALA  |
| 56  | D7    | 15  | THR  |
| 57  | D8    | 32  | LEU  |
| 57  | D8    | 33  | ASN  |
| 57  | D8    | 35  | GLN  |
| 57  | D8    | 64  | TYR  |
| 2   | AB    | 10  | LEU  |
| 2   | AB    | 29  | ALA  |
| 2   | AB    | 30  | ARG  |
| 2   | AB    | 65  | GLY  |
| 2   | AB    | 88  | ALA  |
| 2   | AB    | 152 | PHE  |
| 2   | AB    | 157 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 174 | VAL  |
| 2   | AB    | 208 | ILE  |
| 2   | AB    | 214 | ILE  |
| 2   | AB    | 227 | GLY  |
| 3   | AC    | 3   | ASN  |
| 3   | AC    | 41  | GLY  |
| 3   | AC    | 49  | SER  |
| 3   | AC    | 81  | GLY  |
| 3   | AC    | 160 | ALA  |
| 3   | AC    | 176 | HIS  |
| 4   | AD    | 5   | ILE  |
| 4   | AD    | 124 | GLY  |
| 5   | AE    | 7   | GLU  |
| 5   | AE    | 16  | THR  |
| 5   | AE    | 74  | GLY  |
| 5   | AE    | 103 | GLY  |
| 5   | AE    | 150 | ARG  |
| 6   | AF    | 39  | LYS  |
| 6   | AF    | 78  | GLU  |
| 7   | AG    | 14  | PRO  |
| 7   | AG    | 23  | VAL  |
| 7   | AG    | 128 | ALA  |
| 8   | AH    | 2   | LEU  |
| 9   | AI    | 38  | GLN  |
| 9   | AI    | 41  | VAL  |
| 9   | AI    | 46  | ALA  |
| 9   | AI    | 117 | HIS  |
| 10  | AJ    | 6   | ILE  |
| 10  | AJ    | 82  | ILE  |
| 11  | AK    | 124 | LYS  |
| 12  | AL    | 4   | ILE  |
| 12  | AL    | 9   | ARG  |
| 12  | AL    | 24  | LEU  |
| 12  | AL    | 43  | LYS  |
| 12  | AL    | 59  | SER  |
| 12  | AL    | 113 | SER  |
| 12  | AL    | 114 | ARG  |
| 12  | AL    | 118 | GLY  |
| 13  | AM    | 8   | GLU  |
| 13  | AM    | 15  | VAL  |
| 13  | AM    | 21  | TYR  |
| 13  | AM    | 49  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | AM    | 70  | LEU  |
| 13  | AM    | 83  | ASP  |
| 13  | AM    | 90  | LEU  |
| 13  | AM    | 91  | ARG  |
| 13  | AM    | 100 | GLY  |
| 13  | AM    | 104 | ARG  |
| 13  | AM    | 105 | THR  |
| 13  | AM    | 112 | GLY  |
| 14  | AN    | 23  | ARG  |
| 14  | AN    | 29  | ARG  |
| 14  | AN    | 58  | LYS  |
| 15  | AO    | 86  | GLY  |
| 16  | AP    | 63  | GLY  |
| 17  | AQ    | 79  | SER  |
| 17  | AQ    | 80  | GLY  |
| 17  | AQ    | 82  | MET  |
| 18  | AR    | 23  | LYS  |
| 18  | AR    | 41  | LYS  |
| 18  | AR    | 57  | GLY  |
| 18  | AR    | 61  | LYS  |
| 18  | AR    | 72  | ARG  |
| 20  | AT    | 29  | LYS  |
| 20  | AT    | 48  | LYS  |
| 20  | AT    | 64  | ASP  |
| 20  | AT    | 71  | THR  |
| 20  | AT    | 97  | ALA  |
| 20  | AT    | 99  | LEU  |
| 21  | AU    | 7   | ARG  |
| 29  | BC    | 20  | TYR  |
| 29  | BC    | 48  | GLY  |
| 29  | BC    | 49  | ILE  |
| 29  | BC    | 69  | GLY  |
| 29  | BC    | 76  | ALA  |
| 29  | BC    | 77  | ILE  |
| 29  | BC    | 91  | ALA  |
| 29  | BC    | 109 | ASP  |
| 29  | BC    | 129 | ARG  |
| 29  | BC    | 133 | PRO  |
| 29  | BC    | 151 | GLU  |
| 29  | BC    | 164 | ARG  |
| 29  | BC    | 183 | GLU  |
| 29  | BC    | 201 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BD    | 13  | ARG  |
| 30  | BD    | 27  | THR  |
| 30  | BD    | 34  | VAL  |
| 30  | BD    | 35  | LYS  |
| 30  | BD    | 267 | SER  |
| 31  | BE    | 35  | GLN  |
| 31  | BE    | 59  | VAL  |
| 31  | BE    | 60  | ASN  |
| 31  | BE    | 69  | LYS  |
| 31  | BE    | 76  | ARG  |
| 31  | BE    | 88  | GLY  |
| 31  | BE    | 157 | ALA  |
| 32  | BF    | 7   | TYR  |
| 32  | BF    | 14  | PRO  |
| 32  | BF    | 21  | ALA  |
| 32  | BF    | 57  | VAL  |
| 32  | BF    | 129 | PHE  |
| 32  | BF    | 134 | GLY  |
| 32  | BF    | 146 | ALA  |
| 32  | BF    | 161 | GLU  |
| 32  | BF    | 168 | ARG  |
| 32  | BF    | 188 | ARG  |
| 33  | BG    | 3   | LEU  |
| 33  | BG    | 14  | GLU  |
| 33  | BG    | 86  | MET  |
| 33  | BG    | 153 | ARG  |
| 33  | BG    | 154 | GLY  |
| 34  | BH    | 24  | VAL  |
| 34  | BH    | 91  | GLY  |
| 34  | BH    | 93  | GLY  |
| 34  | BH    | 154 | PRO  |
| 35  | BI    | 15  | VAL  |
| 35  | BI    | 26  | ALA  |
| 35  | BI    | 43  | ASN  |
| 35  | BI    | 49  | ALA  |
| 35  | BI    | 85  | GLU  |
| 35  | BI    | 94  | ALA  |
| 35  | BI    | 111 | PRO  |
| 35  | BI    | 121 | LYS  |
| 35  | BI    | 122 | GLU  |
| 35  | BI    | 131 | LYS  |
| 35  | BI    | 135 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BI    | 139 | GLN  |
| 35  | BI    | 140 | LEU  |
| 35  | BI    | 145 | VAL  |
| 36  | BN    | 37  | LYS  |
| 36  | BN    | 42  | TRP  |
| 36  | BN    | 64  | GLY  |
| 37  | BO    | 52  | VAL  |
| 37  | BO    | 115 | VAL  |
| 38  | BP    | 23  | PRO  |
| 38  | BP    | 30  | THR  |
| 38  | BP    | 34  | GLY  |
| 38  | BP    | 65  | ARG  |
| 38  | BP    | 139 | LYS  |
| 39  | BQ    | 4   | PRO  |
| 39  | BQ    | 13  | GLN  |
| 39  | BQ    | 59  | ARG  |
| 39  | BQ    | 108 | GLY  |
| 40  | BR    | 5   | LYS  |
| 40  | BR    | 23  | ASN  |
| 40  | BR    | 42  | LYS  |
| 40  | BR    | 45  | ARG  |
| 40  | BR    | 82  | GLU  |
| 41  | BS    | 24  | LEU  |
| 41  | BS    | 57  | LYS  |
| 41  | BS    | 85  | VAL  |
| 41  | BS    | 86  | ALA  |
| 41  | BS    | 87  | PHE  |
| 41  | BS    | 89  | ARG  |
| 41  | BS    | 90  | GLY  |
| 41  | BS    | 97  | ARG  |
| 41  | BS    | 104 | GLY  |
| 42  | BT    | 24  | PRO  |
| 42  | BT    | 26  | ASP  |
| 42  | BT    | 29  | ARG  |
| 42  | BT    | 88  | ILE  |
| 42  | BT    | 128 | GLU  |
| 42  | BT    | 132 | LYS  |
| 43  | BU    | 62  | ILE  |
| 43  | BU    | 66  | ASN  |
| 44  | BV    | 18  | LEU  |
| 44  | BV    | 51  | VAL  |
| 44  | BV    | 55  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | BV    | 79  | VAL  |
| 45  | BW    | 15  | ARG  |
| 45  | BW    | 45  | TYR  |
| 45  | BW    | 63  | ASP  |
| 45  | BW    | 110 | LYS  |
| 46  | BX    | 68  | ARG  |
| 47  | BY    | 17  | SER  |
| 47  | BY    | 41  | GLY  |
| 47  | BY    | 44  | ILE  |
| 47  | BY    | 47  | LYS  |
| 47  | BY    | 49  | VAL  |
| 48  | BZ    | 26  | VAL  |
| 48  | BZ    | 110 | VAL  |
| 48  | BZ    | 165 | SER  |
| 49  | B0    | 72  | ARG  |
| 49  | B0    | 73  | GLY  |
| 50  | B1    | 45  | ASN  |
| 50  | B1    | 58  | ILE  |
| 50  | B1    | 85  | LEU  |
| 53  | B4    | 52  | SER  |
| 53  | B4    | 65  | CYS  |
| 54  | B5    | 51  | TYR  |
| 54  | B5    | 57  | VAL  |
| 55  | B6    | 49  | HIS  |
| 56  | B7    | 12  | ARG  |
| 57  | B8    | 11  | LYS  |
| 57  | B8    | 41  | ILE  |
| 57  | B8    | 51  | ALA  |
| 2   | CB    | 32  | ILE  |
| 2   | CB    | 38  | GLY  |
| 2   | CB    | 88  | ALA  |
| 2   | CB    | 150 | SER  |
| 2   | CB    | 153 | ARG  |
| 2   | CB    | 240 | GLN  |
| 3   | CC    | 20  | SER  |
| 3   | CC    | 101 | LEU  |
| 3   | CC    | 145 | GLY  |
| 3   | CC    | 189 | ALA  |
| 4   | CD    | 4   | TYR  |
| 4   | CD    | 9   | CYS  |
| 4   | CD    | 47  | ARG  |
| 4   | CD    | 69  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CD    | 76  | ARG  |
| 4   | CD    | 85  | LYS  |
| 4   | CD    | 88  | VAL  |
| 4   | CD    | 110 | PHE  |
| 4   | CD    | 166 | LYS  |
| 4   | CD    | 171 | GLY  |
| 5   | CE    | 12  | LEU  |
| 5   | CE    | 70  | PRO  |
| 5   | CE    | 85  | GLY  |
| 5   | CE    | 104 | ALA  |
| 6   | CF    | 34  | GLY  |
| 7   | CG    | 116 | ALA  |
| 8   | CH    | 72  | PRO  |
| 8   | CH    | 76  | PRO  |
| 8   | CH    | 121 | ASP  |
| 8   | CH    | 129 | VAL  |
| 9   | CI    | 41  | VAL  |
| 9   | CI    | 61  | ALA  |
| 9   | CI    | 67  | GLY  |
| 9   | CI    | 94  | ALA  |
| 9   | CI    | 100 | GLY  |
| 9   | CI    | 119 | ALA  |
| 9   | CI    | 126 | SER  |
| 10  | CJ    | 23  | ILE  |
| 10  | CJ    | 59  | SER  |
| 10  | CJ    | 88  | LEU  |
| 11  | CK    | 49  | GLY  |
| 12  | CL    | 16  | ARG  |
| 12  | CL    | 62  | GLU  |
| 12  | CL    | 77  | HIS  |
| 12  | CL    | 118 | GLY  |
| 12  | CL    | 124 | GLU  |
| 13  | CM    | 58  | GLU  |
| 13  | CM    | 71  | ARG  |
| 13  | CM    | 81  | LEU  |
| 13  | CM    | 91  | ARG  |
| 13  | CM    | 100 | GLY  |
| 13  | CM    | 106 | ASN  |
| 13  | CM    | 117 | VAL  |
| 14  | CN    | 17  | LYS  |
| 14  | CN    | 23  | ARG  |
| 14  | CN    | 41  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | CN    | 46  | GLU  |
| 15  | CO    | 26  | GLU  |
| 15  | CO    | 86  | GLY  |
| 16  | CP    | 59  | TRP  |
| 16  | CP    | 83  | GLU  |
| 18  | CR    | 27  | GLY  |
| 19  | CS    | 14  | HIS  |
| 19  | CS    | 29  | ARG  |
| 19  | CS    | 70  | LYS  |
| 19  | CS    | 80  | TYR  |
| 20  | CT    | 73  | HIS  |
| 21  | CU    | 3   | LYS  |
| 29  | DC    | 19  | VAL  |
| 29  | DC    | 22  | ILE  |
| 29  | DC    | 43  | VAL  |
| 29  | DC    | 52  | ARG  |
| 29  | DC    | 120 | MET  |
| 29  | DC    | 144 | THR  |
| 29  | DC    | 149 | ILE  |
| 29  | DC    | 152 | ILE  |
| 29  | DC    | 195 | ALA  |
| 29  | DC    | 210 | ARG  |
| 30  | DD    | 3   | VAL  |
| 30  | DD    | 16  | MET  |
| 30  | DD    | 57  | GLY  |
| 30  | DD    | 147 | LEU  |
| 30  | DD    | 191 | ALA  |
| 30  | DD    | 236 | GLY  |
| 30  | DD    | 239 | ARG  |
| 30  | DD    | 268 | ARG  |
| 30  | DD    | 272 | ALA  |
| 31  | DE    | 40  | GLU  |
| 31  | DE    | 53  | PRO  |
| 31  | DE    | 66  | HIS  |
| 31  | DE    | 70  | ALA  |
| 31  | DE    | 72  | VAL  |
| 31  | DE    | 82  | ARG  |
| 31  | DE    | 84  | PHE  |
| 31  | DE    | 94  | GLU  |
| 31  | DE    | 98  | PRO  |
| 31  | DE    | 102 | VAL  |
| 31  | DE    | 112 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | DE    | 113 | PHE  |
| 31  | DE    | 118 | LYS  |
| 31  | DE    | 129 | HIS  |
| 31  | DE    | 130 | GLY  |
| 31  | DE    | 152 | LYS  |
| 31  | DE    | 162 | ALA  |
| 31  | DE    | 169 | ASN  |
| 32  | DF    | 5   | ALA  |
| 32  | DF    | 14  | PRO  |
| 32  | DF    | 21  | ALA  |
| 32  | DF    | 26  | ALA  |
| 32  | DF    | 69  | HIS  |
| 32  | DF    | 78  | ILE  |
| 32  | DF    | 81  | PRO  |
| 32  | DF    | 127 | GLU  |
| 32  | DF    | 134 | GLY  |
| 32  | DF    | 160 | ASN  |
| 33  | DG    | 110 | ALA  |
| 33  | DG    | 112 | PRO  |
| 33  | DG    | 123 | ASN  |
| 33  | DG    | 143 | GLU  |
| 34  | DH    | 21  | PRO  |
| 34  | DH    | 29  | PRO  |
| 34  | DH    | 41  | MET  |
| 34  | DH    | 84  | SER  |
| 34  | DH    | 98  | LEU  |
| 34  | DH    | 151 | ILE  |
| 34  | DH    | 158 | HIS  |
| 34  | DH    | 170 | ARG  |
| 35  | DI    | 21  | VAL  |
| 35  | DI    | 111 | PRO  |
| 36  | DN    | 47  | ALA  |
| 36  | DN    | 49  | GLY  |
| 36  | DN    | 58  | ASP  |
| 36  | DN    | 91  | LEU  |
| 36  | DN    | 105 | GLY  |
| 36  | DN    | 119 | ARG  |
| 37  | DO    | 7   | TYR  |
| 37  | DO    | 26  | LYS  |
| 37  | DO    | 68  | GLU  |
| 37  | DO    | 80  | ASP  |
| 37  | DO    | 98  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DO    | 111 | PHE  |
| 37  | DO    | 120 | GLU  |
| 38  | DP    | 26  | GLY  |
| 38  | DP    | 34  | GLY  |
| 38  | DP    | 48  | PRO  |
| 38  | DP    | 57  | THR  |
| 38  | DP    | 74  | GLU  |
| 38  | DP    | 110 | TYR  |
| 38  | DP    | 132 | LYS  |
| 38  | DP    | 141 | ALA  |
| 38  | DP    | 147 | LEU  |
| 39  | DQ    | 13  | GLN  |
| 39  | DQ    | 30  | GLY  |
| 39  | DQ    | 108 | GLY  |
| 39  | DQ    | 134 | ARG  |
| 39  | DQ    | 137 | TYR  |
| 40  | DR    | 7   | GLY  |
| 40  | DR    | 14  | SER  |
| 40  | DR    | 17  | ARG  |
| 41  | DS    | 14  | VAL  |
| 41  | DS    | 53  | SER  |
| 41  | DS    | 74  | ALA  |
| 41  | DS    | 90  | GLY  |
| 41  | DS    | 96  | GLY  |
| 41  | DS    | 98  | VAL  |
| 41  | DS    | 102 | ALA  |
| 42  | DT    | 10  | VAL  |
| 42  | DT    | 12  | SER  |
| 42  | DT    | 27  | THR  |
| 42  | DT    | 54  | ARG  |
| 42  | DT    | 58  | ASN  |
| 42  | DT    | 80  | SER  |
| 42  | DT    | 87  | ASP  |
| 42  | DT    | 94  | ALA  |
| 42  | DT    | 107 | ASP  |
| 43  | DU    | 7   | GLY  |
| 43  | DU    | 9   | VAL  |
| 43  | DU    | 26  | GLY  |
| 43  | DU    | 32  | PHE  |
| 43  | DU    | 54  | LYS  |
| 43  | DU    | 77  | SER  |
| 43  | DU    | 90  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | DV    | 23  | GLU  |
| 44  | DV    | 40  | LEU  |
| 44  | DV    | 48  | GLY  |
| 44  | DV    | 50  | PRO  |
| 44  | DV    | 67  | GLY  |
| 45  | DW    | 11  | ARG  |
| 45  | DW    | 21  | VAL  |
| 45  | DW    | 56  | ALA  |
| 45  | DW    | 63  | ASP  |
| 45  | DW    | 111 | HIS  |
| 46  | DX    | 4   | ALA  |
| 46  | DX    | 11  | PRO  |
| 46  | DX    | 40  | LYS  |
| 47  | DY    | 9   | LYS  |
| 47  | DY    | 19  | LYS  |
| 47  | DY    | 41  | GLY  |
| 47  | DY    | 47  | LYS  |
| 47  | DY    | 81  | LYS  |
| 47  | DY    | 99  | CYS  |
| 48  | DZ    | 20  | ALA  |
| 48  | DZ    | 108 | ALA  |
| 48  | DZ    | 116 | LEU  |
| 48  | DZ    | 135 | PHE  |
| 48  | DZ    | 164 | VAL  |
| 48  | DZ    | 168 | GLU  |
| 49  | D0    | 33  | ALA  |
| 49  | D0    | 55  | ARG  |
| 49  | D0    | 83  | PRO  |
| 51  | D2    | 14  | ARG  |
| 51  | D2    | 18  | PRO  |
| 51  | D2    | 51  | ARG  |
| 51  | D2    | 57  | ILE  |
| 52  | D3    | 45  | GLY  |
| 55  | D6    | 15  | GLU  |
| 55  | D6    | 31  | PRO  |
| 55  | D6    | 41  | PRO  |
| 57  | D8    | 34  | TRP  |
| 57  | D8    | 40  | GLU  |
| 57  | D8    | 61  | LEU  |
| 2   | AB    | 48  | MET  |
| 2   | AB    | 49  | GLU  |
| 2   | AB    | 74  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 97  | TRP  |
| 2   | AB    | 130 | ARG  |
| 2   | AB    | 183 | PRO  |
| 2   | AB    | 195 | ASP  |
| 3   | AC    | 62  | ASP  |
| 3   | AC    | 144 | SER  |
| 3   | AC    | 146 | ALA  |
| 3   | AC    | 168 | ALA  |
| 3   | AC    | 181 | ASN  |
| 4   | AD    | 39  | PRO  |
| 4   | AD    | 63  | LYS  |
| 4   | AD    | 68  | TYR  |
| 4   | AD    | 99  | SER  |
| 4   | AD    | 149 | ALA  |
| 4   | AD    | 191 | ARG  |
| 4   | AD    | 193 | ASP  |
| 5   | AE    | 73  | ASN  |
| 5   | AE    | 98  | THR  |
| 5   | AE    | 108 | ALA  |
| 5   | AE    | 146 | ALA  |
| 5   | AE    | 154 | GLY  |
| 6   | AF    | 76  | ALA  |
| 6   | AF    | 93  | SER  |
| 7   | AG    | 39  | ALA  |
| 8   | AH    | 98  | LYS  |
| 10  | AJ    | 90  | LEU  |
| 10  | AJ    | 93  | GLY  |
| 11  | AK    | 87  | THR  |
| 12  | AL    | 45  | PRO  |
| 12  | AL    | 72  | HIS  |
| 12  | AL    | 77  | HIS  |
| 12  | AL    | 80  | VAL  |
| 12  | AL    | 102 | TYR  |
| 13  | AM    | 5   | ALA  |
| 13  | AM    | 7   | VAL  |
| 14  | AN    | 44  | LEU  |
| 15  | AO    | 18  | PHE  |
| 15  | AO    | 80  | ALA  |
| 16  | AP    | 31  | LYS  |
| 16  | AP    | 34  | GLU  |
| 16  | AP    | 68  | ASP  |
| 16  | AP    | 70  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | AP    | 71  | ARG  |
| 17  | AQ    | 49  | GLU  |
| 17  | AQ    | 75  | ARG  |
| 19  | AS    | 5   | LEU  |
| 19  | AS    | 29  | ARG  |
| 20  | AT    | 42  | GLN  |
| 21  | AU    | 25  | LYS  |
| 29  | BC    | 37  | PHE  |
| 29  | BC    | 57  | ASN  |
| 29  | BC    | 89  | ALA  |
| 29  | BC    | 122 | ALA  |
| 29  | BC    | 130 | ILE  |
| 29  | BC    | 188 | ASN  |
| 29  | BC    | 196 | LEU  |
| 29  | BC    | 197 | GLU  |
| 29  | BC    | 213 | TYR  |
| 30  | BD    | 202 | LYS  |
| 30  | BD    | 239 | ARG  |
| 30  | BD    | 241 | PRO  |
| 30  | BD    | 244 | ARG  |
| 31  | BE    | 71  | GLY  |
| 31  | BE    | 83  | ASP  |
| 31  | BE    | 84  | PHE  |
| 31  | BE    | 108 | SER  |
| 31  | BE    | 151 | TYR  |
| 32  | BF    | 26  | ALA  |
| 32  | BF    | 158 | THR  |
| 33  | BG    | 112 | PRO  |
| 33  | BG    | 172 | LEU  |
| 34  | BH    | 27  | LYS  |
| 34  | BH    | 29  | PRO  |
| 34  | BH    | 62  | LYS  |
| 35  | BI    | 8   | PRO  |
| 35  | BI    | 11  | ASN  |
| 35  | BI    | 14  | ASP  |
| 35  | BI    | 24  | GLY  |
| 35  | BI    | 86  | THR  |
| 35  | BI    | 88  | ILE  |
| 35  | BI    | 133 | HIS  |
| 36  | BN    | 7   | LYS  |
| 36  | BN    | 40  | PRO  |
| 36  | BN    | 93  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | BN    | 110 | GLY  |
| 37  | BO    | 76  | ALA  |
| 37  | BO    | 89  | ASN  |
| 38  | BP    | 35  | HIS  |
| 38  | BP    | 36  | LYS  |
| 38  | BP    | 64  | LYS  |
| 38  | BP    | 111 | ARG  |
| 38  | BP    | 140 | ALA  |
| 38  | BP    | 144 | GLU  |
| 38  | BP    | 147 | LEU  |
| 39  | BQ    | 5   | ARG  |
| 39  | BQ    | 15  | GLY  |
| 39  | BQ    | 40  | ALA  |
| 39  | BQ    | 80  | GLU  |
| 40  | BR    | 46  | GLY  |
| 40  | BR    | 72  | ASP  |
| 40  | BR    | 73  | VAL  |
| 41  | BS    | 61  | ASN  |
| 41  | BS    | 83  | LYS  |
| 42  | BT    | 68  | TYR  |
| 42  | BT    | 82  | LEU  |
| 42  | BT    | 97  | ALA  |
| 42  | BT    | 123 | GLN  |
| 43  | BU    | 97  | ASP  |
| 45  | BW    | 6   | ILE  |
| 46  | BX    | 19  | ALA  |
| 46  | BX    | 23  | GLU  |
| 47  | BY    | 19  | LYS  |
| 47  | BY    | 82  | PRO  |
| 48  | BZ    | 113 | GLY  |
| 48  | BZ    | 133 | PRO  |
| 49  | B0    | 57  | PHE  |
| 50  | B1    | 74  | VAL  |
| 50  | B1    | 84  | GLY  |
| 51  | B2    | 14  | ARG  |
| 51  | B2    | 15  | LYS  |
| 51  | B2    | 37  | PHE  |
| 51  | B2    | 44  | LEU  |
| 51  | B2    | 48  | HIS  |
| 51  | B2    | 54  | LYS  |
| 54  | B5    | 34  | PRO  |
| 54  | B5    | 47  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | B5    | 56  | LYS  |
| 55  | B6    | 8   | LYS  |
| 55  | B6    | 15  | GLU  |
| 55  | B6    | 28  | ARG  |
| 55  | B6    | 31  | PRO  |
| 56  | B7    | 11  | LYS  |
| 56  | B7    | 23  | ARG  |
| 57  | B8    | 33  | ASN  |
| 2   | CB    | 19  | HIS  |
| 2   | CB    | 27  | LYS  |
| 2   | CB    | 125 | PRO  |
| 2   | CB    | 128 | GLU  |
| 2   | CB    | 196 | LEU  |
| 2   | CB    | 229 | VAL  |
| 2   | CB    | 238 | LEU  |
| 3   | CC    | 4   | LYS  |
| 3   | CC    | 14  | ILE  |
| 3   | CC    | 55  | VAL  |
| 3   | CC    | 62  | ASP  |
| 4   | CD    | 3   | ARG  |
| 4   | CD    | 7   | PRO  |
| 4   | CD    | 26  | CYS  |
| 4   | CD    | 37  | PRO  |
| 4   | CD    | 92  | VAL  |
| 4   | CD    | 131 | ARG  |
| 4   | CD    | 138 | TYR  |
| 4   | CD    | 159 | ARG  |
| 4   | CD    | 165 | MET  |
| 5   | CE    | 16  | THR  |
| 5   | CE    | 37  | ARG  |
| 5   | CE    | 105 | VAL  |
| 5   | CE    | 108 | ALA  |
| 5   | CE    | 153 | LYS  |
| 5   | CE    | 154 | GLY  |
| 7   | CG    | 42  | ILE  |
| 8   | CH    | 49  | GLU  |
| 8   | CH    | 105 | ARG  |
| 9   | CI    | 11  | LYS  |
| 9   | CI    | 39  | GLY  |
| 9   | CI    | 53  | VAL  |
| 9   | CI    | 111 | ARG  |
| 10  | CJ    | 52  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | CK    | 12  | ARG  |
| 11  | CK    | 77  | MET  |
| 12  | CL    | 25  | LYS  |
| 12  | CL    | 88  | LYS  |
| 12  | CL    | 102 | TYR  |
| 13  | CM    | 61  | GLU  |
| 13  | CM    | 109 | THR  |
| 14  | CN    | 25  | VAL  |
| 14  | CN    | 60  | SER  |
| 15  | CO    | 21  | ASP  |
| 15  | CO    | 27  | VAL  |
| 15  | CO    | 76  | GLU  |
| 16  | CP    | 54  | GLU  |
| 16  | CP    | 63  | GLY  |
| 17  | CQ    | 33  | GLY  |
| 17  | CQ    | 49  | GLU  |
| 19  | CS    | 27  | GLU  |
| 20  | CT    | 54  | LYS  |
| 20  | CT    | 95  | ALA  |
| 29  | DC    | 67  | GLY  |
| 29  | DC    | 130 | ILE  |
| 29  | DC    | 132 | GLY  |
| 29  | DC    | 154 | ARG  |
| 29  | DC    | 158 | ALA  |
| 29  | DC    | 170 | ALA  |
| 29  | DC    | 172 | HIS  |
| 30  | DD    | 134 | ARG  |
| 30  | DD    | 140 | THR  |
| 30  | DD    | 150 | LYS  |
| 30  | DD    | 225 | ALA  |
| 31  | DE    | 2   | LYS  |
| 31  | DE    | 27  | LEU  |
| 31  | DE    | 56  | PRO  |
| 31  | DE    | 90  | THR  |
| 31  | DE    | 122 | PHE  |
| 31  | DE    | 151 | TYR  |
| 32  | DF    | 117 | ARG  |
| 32  | DF    | 140 | LEU  |
| 32  | DF    | 150 | GLY  |
| 32  | DF    | 171 | PRO  |
| 33  | DG    | 3   | LEU  |
| 33  | DG    | 4   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | DG    | 10  | LYS  |
| 33  | DG    | 172 | LEU  |
| 34  | DH    | 108 | GLY  |
| 35  | DI    | 14  | ASP  |
| 35  | DI    | 85  | GLU  |
| 35  | DI    | 145 | VAL  |
| 36  | DN    | 11  | PRO  |
| 36  | DN    | 12  | ARG  |
| 36  | DN    | 35  | ARG  |
| 36  | DN    | 40  | PRO  |
| 36  | DN    | 133 | GLN  |
| 36  | DN    | 135 | PRO  |
| 38  | DP    | 14  | LYS  |
| 38  | DP    | 30  | THR  |
| 38  | DP    | 42  | SER  |
| 38  | DP    | 55  | ARG  |
| 38  | DP    | 56  | SER  |
| 38  | DP    | 111 | ARG  |
| 38  | DP    | 145 | PRO  |
| 38  | DP    | 146 | VAL  |
| 39  | DQ    | 4   | PRO  |
| 39  | DQ    | 16  | ARG  |
| 39  | DQ    | 56  | ARG  |
| 39  | DQ    | 85  | LYS  |
| 39  | DQ    | 117 | ALA  |
| 40  | DR    | 94  | TYR  |
| 40  | DR    | 107 | ASP  |
| 41  | DS    | 24  | LEU  |
| 41  | DS    | 42  | ASP  |
| 41  | DS    | 78  | LEU  |
| 41  | DS    | 89  | ARG  |
| 41  | DS    | 93  | LYS  |
| 41  | DS    | 107 | GLU  |
| 42  | DT    | 29  | ARG  |
| 42  | DT    | 31  | SER  |
| 42  | DT    | 61  | PHE  |
| 42  | DT    | 68  | TYR  |
| 43  | DU    | 43  | GLY  |
| 43  | DU    | 63  | VAL  |
| 44  | DV    | 16  | PRO  |
| 45  | DW    | 9   | TYR  |
| 45  | DW    | 40  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | DW    | 80  | PRO  |
| 45  | DW    | 109 | GLU  |
| 46  | DX    | 13  | LEU  |
| 46  | DX    | 60  | ARG  |
| 47  | DY    | 10  | GLY  |
| 47  | DY    | 62  | GLU  |
| 47  | DY    | 67  | LEU  |
| 47  | DY    | 100 | ALA  |
| 48  | DZ    | 107 | PRO  |
| 48  | DZ    | 163 | ALA  |
| 48  | DZ    | 165 | SER  |
| 50  | D1    | 56  | GLN  |
| 50  | D1    | 95  | LEU  |
| 51  | D2    | 17  | SER  |
| 51  | D2    | 23  | LYS  |
| 51  | D2    | 24  | LEU  |
| 51  | D2    | 43  | GLN  |
| 54  | D5    | 10  | LYS  |
| 54  | D5    | 32  | PRO  |
| 55  | D6    | 18  | ARG  |
| 55  | D6    | 28  | ARG  |
| 55  | D6    | 33  | LYS  |
| 55  | D6    | 43  | CYS  |
| 55  | D6    | 44  | ARG  |
| 56  | D7    | 14  | LYS  |
| 57  | D8    | 53  | PRO  |
| 58  | D9    | 31  | LYS  |
| 2   | AB    | 78  | GLN  |
| 2   | AB    | 237 | ALA  |
| 3   | AC    | 20  | SER  |
| 3   | AC    | 107 | GLN  |
| 3   | AC    | 119 | ARG  |
| 4   | AD    | 4   | TYR  |
| 4   | AD    | 42  | GLN  |
| 4   | AD    | 66  | ARG  |
| 4   | AD    | 85  | LYS  |
| 4   | AD    | 91  | SER  |
| 4   | AD    | 206 | PHE  |
| 5   | AE    | 85  | GLY  |
| 5   | AE    | 133 | TYR  |
| 6   | AF    | 17  | SER  |
| 6   | AF    | 84  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | AG    | 6   | ARG  |
| 8   | AH    | 15  | ASN  |
| 8   | AH    | 20  | TYR  |
| 9   | AI    | 49  | PRO  |
| 9   | AI    | 103 | THR  |
| 11  | AK    | 40  | ILE  |
| 11  | AK    | 43  | SER  |
| 11  | AK    | 62  | GLN  |
| 11  | AK    | 106 | LYS  |
| 11  | AK    | 125 | PHE  |
| 12  | AL    | 88  | LYS  |
| 13  | AM    | 48  | LEU  |
| 15  | AO    | 33  | THR  |
| 15  | AO    | 40  | SER  |
| 15  | AO    | 73  | GLU  |
| 15  | AO    | 76  | GLU  |
| 15  | AO    | 88  | ARG  |
| 17  | AQ    | 14  | LYS  |
| 18  | AR    | 60  | ALA  |
| 20  | AT    | 12  | ALA  |
| 20  | AT    | 25  | ARG  |
| 20  | AT    | 65  | LYS  |
| 20  | AT    | 84  | LEU  |
| 20  | AT    | 98  | PRO  |
| 29  | BC    | 35  | ALA  |
| 29  | BC    | 54  | SER  |
| 29  | BC    | 66  | HIS  |
| 30  | BD    | 11  | PRO  |
| 30  | BD    | 12  | SER  |
| 30  | BD    | 28  | GLU  |
| 30  | BD    | 30  | GLU  |
| 30  | BD    | 32  | SER  |
| 30  | BD    | 80  | ALA  |
| 30  | BD    | 108 | PRO  |
| 30  | BD    | 127 | VAL  |
| 30  | BD    | 206 | LEU  |
| 30  | BD    | 238 | GLY  |
| 30  | BD    | 262 | ARG  |
| 31  | BE    | 117 | MET  |
| 32  | BF    | 71  | GLY  |
| 32  | BF    | 131 | GLY  |
| 33  | BG    | 46  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | BG    | 120 | LEU  |
| 34  | BH    | 40  | GLU  |
| 34  | BH    | 41  | MET  |
| 35  | BI    | 12  | LEU  |
| 35  | BI    | 40  | THR  |
| 35  | BI    | 119 | PRO  |
| 35  | BI    | 130 | TYR  |
| 35  | BI    | 132 | PRO  |
| 36  | BN    | 126 | PRO  |
| 37  | BO    | 120 | GLU  |
| 38  | BP    | 48  | PRO  |
| 38  | BP    | 49  | ARG  |
| 38  | BP    | 56  | SER  |
| 38  | BP    | 98  | GLU  |
| 38  | BP    | 110 | TYR  |
| 38  | BP    | 149 | GLU  |
| 39  | BQ    | 133 | ARG  |
| 40  | BR    | 41  | ALA  |
| 40  | BR    | 49  | ASP  |
| 41  | BS    | 14  | VAL  |
| 41  | BS    | 46  | VAL  |
| 41  | BS    | 103 | GLU  |
| 42  | BT    | 20  | PRO  |
| 42  | BT    | 101 | PHE  |
| 43  | BU    | 60  | LEU  |
| 45  | BW    | 37  | ARG  |
| 45  | BW    | 105 | VAL  |
| 46  | BX    | 40  | LYS  |
| 47  | BY    | 11  | ASP  |
| 48  | BZ    | 45  | LYS  |
| 48  | BZ    | 107 | PRO  |
| 48  | BZ    | 171 | ALA  |
| 48  | BZ    | 172 | ALA  |
| 49  | B0    | 35  | ASN  |
| 49  | B0    | 71  | ASP  |
| 51  | B2    | 34  | GLU  |
| 53  | B4    | 54  | LYS  |
| 55  | B6    | 18  | ARG  |
| 55  | B6    | 44  | ARG  |
| 57  | B8    | 31  | HIS  |
| 57  | B8    | 40  | GLU  |
| 2   | CB    | 91  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 106 | LYS  |
| 2   | CB    | 130 | ARG  |
| 2   | CB    | 167 | PRO  |
| 3   | CC    | 46  | GLU  |
| 3   | CC    | 77  | ILE  |
| 3   | CC    | 98  | ASN  |
| 3   | CC    | 195 | VAL  |
| 4   | CD    | 13  | ARG  |
| 4   | CD    | 24  | GLU  |
| 4   | CD    | 80  | GLU  |
| 4   | CD    | 179 | GLU  |
| 5   | CE    | 130 | ASN  |
| 6   | CF    | 43  | LEU  |
| 7   | CG    | 7   | ALA  |
| 8   | CH    | 6   | ILE  |
| 8   | CH    | 73  | ASP  |
| 9   | CI    | 35  | GLU  |
| 9   | CI    | 117 | HIS  |
| 10  | CJ    | 41  | PRO  |
| 10  | CJ    | 86  | MET  |
| 11  | CK    | 50  | TYR  |
| 11  | CK    | 117 | ASN  |
| 12  | CL    | 48  | ALA  |
| 12  | CL    | 72  | HIS  |
| 12  | CL    | 78  | SER  |
| 13  | CM    | 59  | TYR  |
| 13  | CM    | 104 | ARG  |
| 14  | CN    | 19  | ARG  |
| 15  | CO    | 12  | ILE  |
| 15  | CO    | 19  | PRO  |
| 17  | CQ    | 64  | PRO  |
| 18  | CR    | 68  | LYS  |
| 19  | CS    | 12  | ASP  |
| 29  | DC    | 64  | LEU  |
| 29  | DC    | 125 | SER  |
| 29  | DC    | 145 | VAL  |
| 29  | DC    | 161 | ILE  |
| 29  | DC    | 168 | THR  |
| 29  | DC    | 213 | TYR  |
| 30  | DD    | 244 | ARG  |
| 31  | DE    | 204 | ALA  |
| 32  | DF    | 108 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | DF    | 158 | THR  |
| 33  | DG    | 49  | ASP  |
| 33  | DG    | 153 | ARG  |
| 33  | DG    | 179 | PRO  |
| 34  | DH    | 13  | LYS  |
| 34  | DH    | 47  | GLU  |
| 34  | DH    | 53  | GLU  |
| 34  | DH    | 68  | THR  |
| 34  | DH    | 97  | ARG  |
| 35  | DI    | 30  | LEU  |
| 35  | DI    | 83  | ALA  |
| 35  | DI    | 89  | TYR  |
| 36  | DN    | 134 | ARG  |
| 37  | DO    | 5   | GLN  |
| 39  | DQ    | 29  | PHE  |
| 39  | DQ    | 67  | ARG  |
| 40  | DR    | 106 | GLY  |
| 41  | DS    | 18  | ILE  |
| 41  | DS    | 85  | VAL  |
| 41  | DS    | 91  | PRO  |
| 42  | DT    | 4   | GLY  |
| 42  | DT    | 20  | PRO  |
| 42  | DT    | 57  | PHE  |
| 42  | DT    | 88  | ILE  |
| 42  | DT    | 97  | ALA  |
| 43  | DU    | 45  | TYR  |
| 43  | DU    | 111 | GLU  |
| 44  | DV    | 24  | LYS  |
| 44  | DV    | 30  | GLY  |
| 45  | DW    | 75  | TYR  |
| 46  | DX    | 85  | PRO  |
| 47  | DY    | 31  | LEU  |
| 47  | DY    | 39  | VAL  |
| 47  | DY    | 50  | ARG  |
| 47  | DY    | 55  | TYR  |
| 47  | DY    | 66  | PRO  |
| 48  | DZ    | 46  | VAL  |
| 48  | DZ    | 65  | SER  |
| 49  | D0    | 35  | ASN  |
| 50  | D1    | 6   | GLU  |
| 50  | D1    | 45  | ASN  |
| 50  | D1    | 53  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | D4    | 61  | VAL  |
| 54  | D5    | 11  | THR  |
| 54  | D5    | 24  | ALA  |
| 54  | D5    | 33  | CYS  |
| 55  | D6    | 49  | HIS  |
| 57  | D8    | 29  | LYS  |
| 57  | D8    | 37  | SER  |
| 57  | D8    | 54  | GLU  |
| 58  | D9    | 35  | ARG  |
| 2   | AB    | 159 | PRO  |
| 2   | AB    | 191 | ASP  |
| 2   | AB    | 192 | SER  |
| 3   | AC    | 54  | ARG  |
| 4   | AD    | 65  | ARG  |
| 5   | AE    | 27  | ARG  |
| 7   | AG    | 41  | ARG  |
| 7   | AG    | 100 | ALA  |
| 9   | AI    | 82  | ALA  |
| 11  | AK    | 39  | PRO  |
| 12  | AL    | 25  | LYS  |
| 13  | AM    | 81  | LEU  |
| 15  | AO    | 13  | GLN  |
| 15  | AO    | 87  | ILE  |
| 17  | AQ    | 78  | GLU  |
| 18  | AR    | 54  | ARG  |
| 18  | AR    | 55  | ARG  |
| 21  | AU    | 9   | ARG  |
| 29  | BC    | 64  | LEU  |
| 29  | BC    | 78  | ALA  |
| 29  | BC    | 152 | ILE  |
| 29  | BC    | 200 | LYS  |
| 29  | BC    | 215 | THR  |
| 30  | BD    | 23  | GLU  |
| 31  | BE    | 70  | ALA  |
| 32  | BF    | 102 | PRO  |
| 33  | BG    | 142 | PRO  |
| 34  | BH    | 55  | PRO  |
| 35  | BI    | 17  | GLN  |
| 35  | BI    | 101 | LEU  |
| 36  | BN    | 57  | ALA  |
| 36  | BN    | 127 | ASP  |
| 39  | BQ    | 28  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BQ    | 119 | ARG  |
| 41  | BS    | 21  | THR  |
| 42  | BT    | 32  | TYR  |
| 43  | BU    | 92  | ARG  |
| 44  | BV    | 53  | GLU  |
| 45  | BW    | 93  | ALA  |
| 47  | BY    | 57  | GLN  |
| 47  | BY    | 67  | LEU  |
| 47  | BY    | 81  | LYS  |
| 48  | BZ    | 163 | ALA  |
| 48  | BZ    | 173 | VAL  |
| 49  | B0    | 74  | ARG  |
| 50  | B1    | 37  | ILE  |
| 52  | B3    | 41  | PRO  |
| 56  | B7    | 46  | VAL  |
| 2   | CB    | 96  | ARG  |
| 2   | CB    | 169 | LYS  |
| 3   | CC    | 22  | TRP  |
| 4   | CD    | 5   | ILE  |
| 5   | CE    | 8   | GLU  |
| 7   | CG    | 33  | ASP  |
| 8   | CH    | 30  | ARG  |
| 8   | CH    | 68  | ARG  |
| 8   | CH    | 87  | SER  |
| 8   | CH    | 107 | LEU  |
| 10  | CJ    | 27  | ALA  |
| 12  | CL    | 73  | ASN  |
| 13  | CM    | 36  | LYS  |
| 13  | CM    | 116 | THR  |
| 14  | CN    | 59  | ALA  |
| 15  | CO    | 46  | HIS  |
| 16  | CP    | 28  | ARG  |
| 16  | CP    | 46  | PRO  |
| 18  | CR    | 36  | ASN  |
| 18  | CR    | 71  | LYS  |
| 29  | DC    | 54  | SER  |
| 29  | DC    | 57  | ASN  |
| 29  | DC    | 71  | GLN  |
| 29  | DC    | 78  | ALA  |
| 29  | DC    | 175 | VAL  |
| 30  | DD    | 11  | PRO  |
| 30  | DD    | 35  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DD    | 44  | ASN  |
| 32  | DF    | 9   | ILE  |
| 32  | DF    | 70  | THR  |
| 32  | DF    | 84  | VAL  |
| 32  | DF    | 161 | GLU  |
| 32  | DF    | 178 | PRO  |
| 33  | DG    | 86  | MET  |
| 34  | DH    | 45  | VAL  |
| 34  | DH    | 85  | LYS  |
| 34  | DH    | 154 | PRO  |
| 35  | DI    | 71  | ILE  |
| 35  | DI    | 87  | LYS  |
| 35  | DI    | 133 | HIS  |
| 36  | DN    | 5   | VAL  |
| 36  | DN    | 94  | HIS  |
| 37  | DO    | 14  | THR  |
| 37  | DO    | 93  | PRO  |
| 37  | DO    | 112 | MET  |
| 38  | DP    | 25  | SER  |
| 38  | DP    | 40  | SER  |
| 40  | DR    | 10  | LEU  |
| 40  | DR    | 90  | ARG  |
| 40  | DR    | 93  | GLY  |
| 41  | DS    | 22  | GLY  |
| 42  | DT    | 3   | ARG  |
| 42  | DT    | 35  | LYS  |
| 42  | DT    | 102 | ILE  |
| 43  | DU    | 65  | ILE  |
| 44  | DV    | 22  | VAL  |
| 44  | DV    | 35  | LEU  |
| 44  | DV    | 38  | LEU  |
| 47  | DY    | 17  | SER  |
| 47  | DY    | 27  | VAL  |
| 47  | DY    | 57  | GLN  |
| 47  | DY    | 96  | ILE  |
| 48  | DZ    | 38  | VAL  |
| 50  | D1    | 27  | GLU  |
| 50  | D1    | 52  | ARG  |
| 53  | D4    | 54  | LYS  |
| 57  | D8    | 18  | ALA  |
| 57  | D8    | 51  | ALA  |
| 2   | AB    | 143 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 96  | GLY  |
| 4   | AD    | 88  | VAL  |
| 4   | AD    | 129 | ASN  |
| 4   | AD    | 164 | ALA  |
| 4   | AD    | 196 | LEU  |
| 9   | AI    | 97  | LYS  |
| 12  | AL    | 11  | GLY  |
| 12  | AL    | 16  | ARG  |
| 16  | AP    | 28  | ARG  |
| 17  | AQ    | 17  | LYS  |
| 17  | AQ    | 66  | SER  |
| 19  | AS    | 26  | GLY  |
| 20  | AT    | 78  | ALA  |
| 20  | AT    | 96  | GLY  |
| 29  | BC    | 44  | HIS  |
| 29  | BC    | 50  | ASP  |
| 29  | BC    | 203 | GLY  |
| 31  | BE    | 45  | THR  |
| 31  | BE    | 66  | HIS  |
| 32  | BF    | 89  | VAL  |
| 32  | BF    | 178 | PRO  |
| 33  | BG    | 144 | ILE  |
| 35  | BI    | 89  | TYR  |
| 37  | BO    | 26  | LYS  |
| 37  | BO    | 48  | PRO  |
| 37  | BO    | 107 | ARG  |
| 40  | BR    | 39  | PRO  |
| 40  | BR    | 92  | GLY  |
| 42  | BT    | 56  | GLY  |
| 42  | BT    | 135 | ALA  |
| 43  | BU    | 25  | TRP  |
| 47  | BY    | 55  | TYR  |
| 48  | BZ    | 135 | PHE  |
| 48  | BZ    | 164 | VAL  |
| 54  | B5    | 50  | GLY  |
| 2   | CB    | 183 | PRO  |
| 2   | CB    | 237 | ALA  |
| 3   | CC    | 72  | LYS  |
| 3   | CC    | 197 | GLY  |
| 5   | CE    | 22  | GLY  |
| 6   | CF    | 33  | TYR  |
| 7   | CG    | 100 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | CG    | 112 | PRO  |
| 8   | CH    | 53  | VAL  |
| 9   | CI    | 123 | PRO  |
| 11  | CK    | 54  | ARG  |
| 11  | CK    | 90  | GLY  |
| 12  | CL    | 9   | ARG  |
| 12  | CL    | 24  | LEU  |
| 19  | CS    | 17  | GLU  |
| 20  | CT    | 23  | ARG  |
| 29  | DC    | 200 | LYS  |
| 30  | DD    | 200 | ASP  |
| 33  | DG    | 14  | GLU  |
| 35  | DI    | 15  | VAL  |
| 35  | DI    | 37  | VAL  |
| 36  | DN    | 81  | GLY  |
| 37  | DO    | 102 | VAL  |
| 38  | DP    | 115 | LEU  |
| 38  | DP    | 144 | GLU  |
| 40  | DR    | 85  | PRO  |
| 42  | DT    | 92  | GLY  |
| 43  | DU    | 15  | LYS  |
| 46  | DX    | 94  | GLY  |
| 49  | D0    | 30  | VAL  |
| 50  | D1    | 30  | VAL  |
| 50  | D1    | 76  | ARG  |
| 56  | D7    | 32  | LYS  |
| 57  | D8    | 3   | LYS  |
| 57  | D8    | 14  | VAL  |
| 58  | D9    | 30  | PRO  |
| 2   | AB    | 167 | PRO  |
| 3   | AC    | 141 | VAL  |
| 3   | AC    | 207 | VAL  |
| 7   | AG    | 34  | GLY  |
| 8   | AH    | 75  | ARG  |
| 8   | AH    | 129 | VAL  |
| 10  | AJ    | 23  | ILE  |
| 16  | AP    | 78  | GLY  |
| 29  | BC    | 43  | VAL  |
| 29  | BC    | 161 | ILE  |
| 29  | BC    | 175 | VAL  |
| 31  | BE    | 29  | GLY  |
| 32  | BF    | 9   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | BF    | 66  | PRO  |
| 32  | BF    | 171 | PRO  |
| 35  | BI    | 134 | PRO  |
| 38  | BP    | 146 | VAL  |
| 43  | BU    | 65  | ILE  |
| 46  | BX    | 94  | GLY  |
| 47  | BY    | 37  | VAL  |
| 2   | CB    | 80  | ILE  |
| 4   | CD    | 29  | PRO  |
| 7   | CG    | 81  | GLY  |
| 18  | CR    | 70  | ILE  |
| 20  | CT    | 33  | ILE  |
| 29  | DC    | 74  | VAL  |
| 29  | DC    | 140 | PRO  |
| 29  | DC    | 212 | VAL  |
| 30  | DD    | 108 | PRO  |
| 30  | DD    | 232 | PRO  |
| 31  | DE    | 39  | PRO  |
| 34  | DH    | 66  | GLY  |
| 39  | DQ    | 100 | GLY  |
| 44  | DV    | 47  | VAL  |
| 45  | DW    | 91  | GLY  |
| 47  | DY    | 98  | VAL  |
| 48  | DZ    | 158 | PRO  |
| 49  | D0    | 47  | PRO  |
| 4   | AD    | 69  | GLY  |
| 18  | AR    | 22  | VAL  |
| 29  | BC    | 58  | VAL  |
| 29  | BC    | 145 | VAL  |
| 31  | BE    | 52  | LEU  |
| 32  | BF    | 126 | VAL  |
| 36  | BN    | 135 | PRO  |
| 44  | BV    | 99  | ILE  |
| 48  | BZ    | 21  | GLY  |
| 48  | BZ    | 138 | VAL  |
| 6   | CF    | 11  | ASN  |
| 9   | CI    | 21  | PRO  |
| 10  | CJ    | 24  | VAL  |
| 10  | CJ    | 75  | ILE  |
| 12  | CL    | 22  | PRO  |
| 12  | CL    | 84  | GLY  |
| 31  | DE    | 9   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | DG    | 109 | VAL  |
| 33  | DG    | 159 | VAL  |
| 37  | DO    | 52  | VAL  |
| 38  | DP    | 7   | ARG  |
| 46  | DX    | 39  | ILE  |
| 47  | DY    | 38  | ILE  |
| 49  | D0    | 6   | GLY  |
| 54  | D5    | 31  | VAL  |
| 2   | AB    | 172 | ILE  |
| 3   | AC    | 74  | GLY  |
| 6   | AF    | 40  | VAL  |
| 12  | AL    | 91  | PRO  |
| 13  | AM    | 38  | GLY  |
| 13  | AM    | 41  | PRO  |
| 16  | AP    | 62  | VAL  |
| 29  | BC    | 65  | PRO  |
| 29  | BC    | 90  | GLY  |
| 33  | BG    | 140 | ILE  |
| 35  | BI    | 84  | GLY  |
| 36  | BN    | 54  | VAL  |
| 38  | BP    | 116 | GLY  |
| 43  | BU    | 102 | GLU  |
| 44  | BV    | 48  | GLY  |
| 47  | BY    | 27  | VAL  |
| 48  | BZ    | 36  | VAL  |
| 48  | BZ    | 157 | PRO  |
| 53  | B4    | 55  | PRO  |
| 3   | CC    | 141 | VAL  |
| 7   | CG    | 88  | PRO  |
| 16  | CP    | 33  | ILE  |
| 17  | CQ    | 28  | PRO  |
| 32  | DF    | 102 | PRO  |
| 32  | DF    | 131 | GLY  |
| 33  | DG    | 122 | PRO  |
| 34  | DH    | 17  | VAL  |
| 36  | DN    | 16  | ILE  |
| 39  | DQ    | 126 | PRO  |
| 40  | DR    | 66  | VAL  |
| 48  | DZ    | 173 | VAL  |
| 3   | AC    | 55  | VAL  |
| 3   | AC    | 114 | PRO  |
| 4   | AD    | 92  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | BF    | 64  | ILE  |
| 32  | BF    | 207 | GLY  |
| 33  | BG    | 70  | VAL  |
| 38  | BP    | 97  | PRO  |
| 42  | BT    | 25  | GLY  |
| 47  | BY    | 39  | VAL  |
| 55  | B6    | 41  | PRO  |
| 2   | CB    | 93  | VAL  |
| 13  | CM    | 85  | GLY  |
| 29  | DC    | 65  | PRO  |
| 30  | DD    | 127 | VAL  |
| 33  | DG    | 127 | GLY  |
| 36  | DN    | 78  | TYR  |
| 40  | DR    | 38  | VAL  |
| 42  | DT    | 42  | ILE  |
| 48  | DZ    | 115 | VAL  |
| 2   | AB    | 202 | PRO  |
| 4   | AD    | 204 | ILE  |
| 10  | AJ    | 36  | GLY  |
| 29  | BC    | 171 | ILE  |
| 33  | BG    | 63  | ILE  |
| 36  | BN    | 36  | GLY  |
| 38  | BP    | 63  | PRO  |
| 41  | BS    | 98  | VAL  |
| 2   | CB    | 72  | GLY  |
| 13  | CM    | 4   | ILE  |
| 13  | CM    | 6   | GLY  |
| 34  | DH    | 39  | PRO  |
| 34  | DH    | 44  | VAL  |
| 35  | DI    | 7   | GLU  |
| 48  | DZ    | 160 | VAL  |
| 36  | DN    | 126 | PRO  |
| 30  | BD    | 245 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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    | 202/220 (92%)  | 169 (84%) | 33 (16%) | 3           | 13 |
| 2   | CB    | 202/220 (92%)  | 174 (86%) | 28 (14%) | 4           | 18 |
| 3   | AC    | 160/188 (85%)  | 129 (81%) | 31 (19%) | 1           | 9  |
| 3   | CC    | 160/188 (85%)  | 140 (88%) | 20 (12%) | 5           | 23 |
| 4   | AD    | 180/181 (99%)  | 147 (82%) | 33 (18%) | 2           | 10 |
| 4   | CD    | 180/181 (99%)  | 147 (82%) | 33 (18%) | 2           | 10 |
| 5   | AE    | 115/123 (94%)  | 101 (88%) | 14 (12%) | 6           | 24 |
| 5   | CE    | 115/123 (94%)  | 96 (84%)  | 19 (16%) | 2           | 13 |
| 6   | AF    | 90/90 (100%)   | 80 (89%)  | 10 (11%) | 7           | 28 |
| 6   | CF    | 90/90 (100%)   | 78 (87%)  | 12 (13%) | 4           | 20 |
| 7   | AG    | 126/127 (99%)  | 106 (84%) | 20 (16%) | 3           | 14 |
| 7   | CG    | 126/127 (99%)  | 106 (84%) | 20 (16%) | 3           | 14 |
| 8   | AH    | 119/119 (100%) | 96 (81%)  | 23 (19%) | 1           | 9  |
| 8   | CH    | 119/119 (100%) | 105 (88%) | 14 (12%) | 6           | 25 |
| 9   | AI    | 97/99 (98%)    | 80 (82%)  | 17 (18%) | 2           | 11 |
| 9   | CI    | 97/99 (98%)    | 85 (88%)  | 12 (12%) | 5           | 23 |
| 10  | AJ    | 88/92 (96%)    | 68 (77%)  | 20 (23%) | 1           | 5  |
| 10  | CJ    | 88/92 (96%)    | 74 (84%)  | 14 (16%) | 3           | 14 |
| 11  | AK    | 90/99 (91%)    | 74 (82%)  | 16 (18%) | 2           | 11 |
| 11  | CK    | 90/99 (91%)    | 78 (87%)  | 12 (13%) | 4           | 20 |
| 12  | AL    | 104/109 (95%)  | 87 (84%)  | 17 (16%) | 3           | 13 |
| 12  | CL    | 104/109 (95%)  | 90 (86%)  | 14 (14%) | 4           | 19 |
| 13  | AM    | 94/101 (93%)   | 75 (80%)  | 19 (20%) | 1           | 7  |
| 13  | CM    | 88/101 (87%)   | 69 (78%)  | 19 (22%) | 1           | 6  |
| 14  | AN    | 49/50 (98%)    | 39 (80%)  | 10 (20%) | 1           | 7  |
| 14  | CN    | 49/50 (98%)    | 37 (76%)  | 12 (24%) | 1           | 3  |
| 15  | AO    | 79/80 (99%)    | 63 (80%)  | 16 (20%) | 1           | 7  |
| 15  | CO    | 79/80 (99%)    | 65 (82%)  | 14 (18%) | 2           | 11 |
| 16  | AP    | 72/74 (97%)    | 63 (88%)  | 9 (12%)  | 5           | 23 |
| 16  | CP    | 72/74 (97%)    | 60 (83%)  | 12 (17%) | 2           | 13 |
| 17  | AQ    | 94/97 (97%)    | 80 (85%)  | 14 (15%) | 3           | 16 |
| 17  | CQ    | 94/97 (97%)    | 84 (89%)  | 10 (11%) | 8           | 30 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 18  | AR    | 61/77 (79%)    | 53 (87%)  | 8 (13%)  | 5           | 21  |
| 18  | CR    | 61/77 (79%)    | 55 (90%)  | 6 (10%)  | 9           | 34  |
| 19  | AS    | 69/80 (86%)    | 53 (77%)  | 16 (23%) | 1           | 4   |
| 19  | CS    | 69/80 (86%)    | 51 (74%)  | 18 (26%) | 0           | 3   |
| 20  | AT    | 76/82 (93%)    | 63 (83%)  | 13 (17%) | 2           | 12  |
| 20  | CT    | 76/82 (93%)    | 65 (86%)  | 11 (14%) | 4           | 17  |
| 21  | AU    | 19/22 (86%)    | 16 (84%)  | 3 (16%)  | 3           | 14  |
| 21  | CU    | 19/22 (86%)    | 18 (95%)  | 1 (5%)   | 26          | 65  |
| 26  | AZ    | 2/2 (100%)     | 2 (100%)  | 0        | 100         | 100 |
| 26  | CZ    | 2/2 (100%)     | 2 (100%)  | 0        | 100         | 100 |
| 29  | BC    | 61/181 (34%)   | 56 (92%)  | 5 (8%)   | 13          | 44  |
| 29  | DC    | 61/181 (34%)   | 51 (84%)  | 10 (16%) | 2           | 13  |
| 30  | BD    | 213/218 (98%)  | 162 (76%) | 51 (24%) | 1           | 4   |
| 30  | DD    | 213/218 (98%)  | 173 (81%) | 40 (19%) | 2           | 10  |
| 31  | BE    | 165/166 (99%)  | 127 (77%) | 38 (23%) | 1           | 4   |
| 31  | DE    | 165/166 (99%)  | 121 (73%) | 44 (27%) | 0           | 3   |
| 32  | BF    | 165/166 (99%)  | 136 (82%) | 29 (18%) | 2           | 11  |
| 32  | DF    | 165/166 (99%)  | 138 (84%) | 27 (16%) | 2           | 13  |
| 33  | BG    | 155/156 (99%)  | 117 (76%) | 38 (24%) | 1           | 3   |
| 33  | DG    | 155/156 (99%)  | 125 (81%) | 30 (19%) | 1           | 9   |
| 34  | BH    | 136/148 (92%)  | 111 (82%) | 25 (18%) | 2           | 10  |
| 34  | DH    | 132/148 (89%)  | 111 (84%) | 21 (16%) | 3           | 14  |
| 35  | BI    | 102/124 (82%)  | 79 (78%)  | 23 (22%) | 1           | 5   |
| 35  | DI    | 103/124 (83%)  | 85 (82%)  | 18 (18%) | 2           | 11  |
| 36  | BN    | 117/119 (98%)  | 88 (75%)  | 29 (25%) | 1           | 3   |
| 36  | DN    | 117/119 (98%)  | 92 (79%)  | 25 (21%) | 1           | 6   |
| 37  | BO    | 100/100 (100%) | 81 (81%)  | 19 (19%) | 2           | 9   |
| 37  | DO    | 100/100 (100%) | 75 (75%)  | 25 (25%) | 1           | 3   |
| 38  | BP    | 112/116 (97%)  | 76 (68%)  | 36 (32%) | 0           | 1   |
| 38  | DP    | 112/116 (97%)  | 79 (70%)  | 33 (30%) | 0           | 2   |
| 39  | BQ    | 111/111 (100%) | 85 (77%)  | 26 (23%) | 1           | 4   |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 39  | DQ    | 110/111 (99%) | 91 (83%)  | 19 (17%) | 2           | 12 |
| 40  | BR    | 100/101 (99%) | 77 (77%)  | 23 (23%) | 1           | 4  |
| 40  | DR    | 100/101 (99%) | 67 (67%)  | 33 (33%) | 0           | 1  |
| 41  | BS    | 77/88 (88%)   | 60 (78%)  | 17 (22%) | 1           | 5  |
| 41  | DS    | 76/88 (86%)   | 62 (82%)  | 14 (18%) | 2           | 10 |
| 42  | BT    | 120/127 (94%) | 81 (68%)  | 39 (32%) | 0           | 1  |
| 42  | DT    | 120/127 (94%) | 88 (73%)  | 32 (27%) | 0           | 3  |
| 43  | BU    | 92/94 (98%)   | 71 (77%)  | 21 (23%) | 1           | 5  |
| 43  | DU    | 92/94 (98%)   | 81 (88%)  | 11 (12%) | 6           | 25 |
| 44  | BV    | 82/82 (100%)  | 59 (72%)  | 23 (28%) | 0           | 2  |
| 44  | DV    | 82/82 (100%)  | 60 (73%)  | 22 (27%) | 0           | 3  |
| 45  | BW    | 91/92 (99%)   | 74 (81%)  | 17 (19%) | 2           | 10 |
| 45  | DW    | 91/92 (99%)   | 72 (79%)  | 19 (21%) | 1           | 6  |
| 46  | BX    | 74/78 (95%)   | 60 (81%)  | 14 (19%) | 2           | 9  |
| 46  | DX    | 74/78 (95%)   | 58 (78%)  | 16 (22%) | 1           | 6  |
| 47  | BY    | 84/91 (92%)   | 62 (74%)  | 22 (26%) | 0           | 3  |
| 47  | DY    | 84/91 (92%)   | 63 (75%)  | 21 (25%) | 1           | 3  |
| 48  | BZ    | 155/179 (87%) | 127 (82%) | 28 (18%) | 2           | 10 |
| 48  | DZ    | 155/179 (87%) | 135 (87%) | 20 (13%) | 5           | 22 |
| 49  | B0    | 66/67 (98%)   | 53 (80%)  | 13 (20%) | 1           | 8  |
| 49  | D0    | 66/67 (98%)   | 58 (88%)  | 8 (12%)  | 6           | 24 |
| 50  | B1    | 74/83 (89%)   | 56 (76%)  | 18 (24%) | 1           | 4  |
| 50  | D1    | 78/83 (94%)   | 63 (81%)  | 15 (19%) | 1           | 9  |
| 51  | B2    | 66/67 (98%)   | 50 (76%)  | 16 (24%) | 1           | 4  |
| 51  | D2    | 66/67 (98%)   | 53 (80%)  | 13 (20%) | 1           | 8  |
| 52  | B3    | 51/52 (98%)   | 42 (82%)  | 9 (18%)  | 2           | 11 |
| 52  | D3    | 51/52 (98%)   | 44 (86%)  | 7 (14%)  | 4           | 19 |
| 53  | B4    | 27/63 (43%)   | 23 (85%)  | 4 (15%)  | 3           | 16 |
| 53  | D4    | 27/63 (43%)   | 25 (93%)  | 2 (7%)   | 16          | 49 |
| 54  | B5    | 51/52 (98%)   | 39 (76%)  | 12 (24%) | 1           | 4  |
| 54  | D5    | 51/52 (98%)   | 42 (82%)  | 9 (18%)  | 2           | 11 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 55  | B6    | 43/52 (83%)      | 30 (70%)   | 13 (30%)   | 0           | 2  |
| 55  | D6    | 44/52 (85%)      | 28 (64%)   | 16 (36%)   | 0           | 1  |
| 56  | B7    | 41/42 (98%)      | 34 (83%)   | 7 (17%)    | 2           | 12 |
| 56  | D7    | 41/42 (98%)      | 36 (88%)   | 5 (12%)    | 6           | 24 |
| 57  | B8    | 53/55 (96%)      | 44 (83%)   | 9 (17%)    | 2           | 12 |
| 57  | D8    | 53/55 (96%)      | 39 (74%)   | 14 (26%)   | 0           | 3  |
| 58  | B9    | 33/34 (97%)      | 24 (73%)   | 9 (27%)    | 0           | 2  |
| 58  | D9    | 33/34 (97%)      | 28 (85%)   | 5 (15%)    | 3           | 16 |
| All | All   | 9600/10432 (92%) | 7750 (81%) | 1850 (19%) | 1           | 9  |

All (1850) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 8   | LYS  |
| 2   | AB    | 15  | VAL  |
| 2   | AB    | 16  | HIS  |
| 2   | AB    | 17  | PHE  |
| 2   | AB    | 36  | ARG  |
| 2   | AB    | 44  | LEU  |
| 2   | AB    | 45  | GLN  |
| 2   | AB    | 53  | ARG  |
| 2   | AB    | 61  | LEU  |
| 2   | AB    | 64  | ARG  |
| 2   | AB    | 69  | LEU  |
| 2   | AB    | 74  | LYS  |
| 2   | AB    | 78  | GLN  |
| 2   | AB    | 80  | ILE  |
| 2   | AB    | 110 | GLN  |
| 2   | AB    | 113 | HIS  |
| 2   | AB    | 130 | ARG  |
| 2   | AB    | 137 | ARG  |
| 2   | AB    | 153 | ARG  |
| 2   | AB    | 155 | LEU  |
| 2   | AB    | 165 | VAL  |
| 2   | AB    | 175 | ARG  |
| 2   | AB    | 178 | ARG  |
| 2   | AB    | 183 | PRO  |
| 2   | AB    | 189 | ASP  |
| 2   | AB    | 196 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 198 | ASP  |
| 2   | AB    | 204 | ASN  |
| 2   | AB    | 206 | ASP  |
| 2   | AB    | 212 | GLN  |
| 2   | AB    | 213 | LEU  |
| 2   | AB    | 215 | LEU  |
| 2   | AB    | 238 | LEU  |
| 3   | AC    | 3   | ASN  |
| 3   | AC    | 5   | ILE  |
| 3   | AC    | 10  | PHE  |
| 3   | AC    | 11  | ARG  |
| 3   | AC    | 12  | LEU  |
| 3   | AC    | 16  | ARG  |
| 3   | AC    | 17  | ASP  |
| 3   | AC    | 21  | ARG  |
| 3   | AC    | 28  | GLN  |
| 3   | AC    | 29  | TYR  |
| 3   | AC    | 31  | HIS  |
| 3   | AC    | 36  | ASP  |
| 3   | AC    | 47  | LEU  |
| 3   | AC    | 52  | LEU  |
| 3   | AC    | 62  | ASP  |
| 3   | AC    | 63  | ASN  |
| 3   | AC    | 76  | VAL  |
| 3   | AC    | 77  | ILE  |
| 3   | AC    | 79  | ARG  |
| 3   | AC    | 94  | LEU  |
| 3   | AC    | 124 | ILE  |
| 3   | AC    | 151 | VAL  |
| 3   | AC    | 154 | SER  |
| 3   | AC    | 165 | THR  |
| 3   | AC    | 178 | LEU  |
| 3   | AC    | 192 | THR  |
| 3   | AC    | 193 | TYR  |
| 3   | AC    | 195 | VAL  |
| 3   | AC    | 198 | VAL  |
| 3   | AC    | 201 | TYR  |
| 3   | AC    | 204 | LEU  |
| 4   | AD    | 3   | ARG  |
| 4   | AD    | 9   | CYS  |
| 4   | AD    | 10  | ARG  |
| 4   | AD    | 11  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AD    | 12  | CYS  |
| 4   | AD    | 15  | GLU  |
| 4   | AD    | 25  | ARG  |
| 4   | AD    | 26  | CYS  |
| 4   | AD    | 28  | SER  |
| 4   | AD    | 31  | CYS  |
| 4   | AD    | 42  | GLN  |
| 4   | AD    | 50  | ARG  |
| 4   | AD    | 58  | LEU  |
| 4   | AD    | 72  | GLU  |
| 4   | AD    | 86  | LYS  |
| 4   | AD    | 92  | VAL  |
| 4   | AD    | 96  | LEU  |
| 4   | AD    | 98  | GLU  |
| 4   | AD    | 101 | LEU  |
| 4   | AD    | 118 | ARG  |
| 4   | AD    | 120 | LEU  |
| 4   | AD    | 122 | ARG  |
| 4   | AD    | 131 | ARG  |
| 4   | AD    | 135 | LEU  |
| 4   | AD    | 139 | ARG  |
| 4   | AD    | 146 | ILE  |
| 4   | AD    | 150 | GLU  |
| 4   | AD    | 161 | ASN  |
| 4   | AD    | 168 | ARG  |
| 4   | AD    | 188 | LEU  |
| 4   | AD    | 196 | LEU  |
| 4   | AD    | 208 | SER  |
| 4   | AD    | 209 | ARG  |
| 5   | AE    | 5   | ASP  |
| 5   | AE    | 10  | MET  |
| 5   | AE    | 16  | THR  |
| 5   | AE    | 20  | GLN  |
| 5   | AE    | 31  | LEU  |
| 5   | AE    | 43  | LEU  |
| 5   | AE    | 64  | ARG  |
| 5   | AE    | 73  | ASN  |
| 5   | AE    | 75  | THR  |
| 5   | AE    | 91  | LEU  |
| 5   | AE    | 101 | ILE  |
| 5   | AE    | 133 | TYR  |
| 5   | AE    | 141 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AE    | 147 | ASP  |
| 6   | AF    | 6   | VAL  |
| 6   | AF    | 10  | LEU  |
| 6   | AF    | 15  | ASP  |
| 6   | AF    | 16  | GLN  |
| 6   | AF    | 43  | LEU  |
| 6   | AF    | 55  | ASP  |
| 6   | AF    | 64  | GLN  |
| 6   | AF    | 80  | ARG  |
| 6   | AF    | 94  | GLN  |
| 6   | AF    | 98  | LEU  |
| 7   | AG    | 5   | ARG  |
| 7   | AG    | 21  | VAL  |
| 7   | AG    | 45  | ASP  |
| 7   | AG    | 57  | GLU  |
| 7   | AG    | 59  | LEU  |
| 7   | AG    | 61  | VAL  |
| 7   | AG    | 68  | ASN  |
| 7   | AG    | 78  | ARG  |
| 7   | AG    | 79  | ARG  |
| 7   | AG    | 89  | MET  |
| 7   | AG    | 92  | SER  |
| 7   | AG    | 104 | LEU  |
| 7   | AG    | 109 | ASN  |
| 7   | AG    | 114 | ARG  |
| 7   | AG    | 118 | VAL  |
| 7   | AG    | 141 | VAL  |
| 7   | AG    | 142 | GLU  |
| 7   | AG    | 143 | ARG  |
| 7   | AG    | 151 | TYR  |
| 7   | AG    | 156 | TRP  |
| 8   | AH    | 1   | MET  |
| 8   | AH    | 4   | ASP  |
| 8   | AH    | 19  | VAL  |
| 8   | AH    | 25  | ASP  |
| 8   | AH    | 26  | VAL  |
| 8   | AH    | 30  | ARG  |
| 8   | AH    | 41  | ARG  |
| 8   | AH    | 52  | ASP  |
| 8   | AH    | 63  | LEU  |
| 8   | AH    | 65  | TYR  |
| 8   | AH    | 75  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | AH    | 78  | GLN  |
| 8   | AH    | 84  | ARG  |
| 8   | AH    | 85  | ARG  |
| 8   | AH    | 87  | SER  |
| 8   | AH    | 91  | ARG  |
| 8   | AH    | 103 | VAL  |
| 8   | AH    | 104 | ARG  |
| 8   | AH    | 107 | LEU  |
| 8   | AH    | 112 | LEU  |
| 8   | AH    | 118 | VAL  |
| 8   | AH    | 119 | LEU  |
| 8   | AH    | 133 | LEU  |
| 9   | AI    | 4   | TYR  |
| 9   | AI    | 10  | ARG  |
| 9   | AI    | 38  | GLN  |
| 9   | AI    | 41  | VAL  |
| 9   | AI    | 54  | ASP  |
| 9   | AI    | 62  | TYR  |
| 9   | AI    | 66  | ARG  |
| 9   | AI    | 78  | LYS  |
| 9   | AI    | 85  | LEU  |
| 9   | AI    | 91  | ASP  |
| 9   | AI    | 95  | LYS  |
| 9   | AI    | 102 | LEU  |
| 9   | AI    | 108 | VAL  |
| 9   | AI    | 114 | TYR  |
| 9   | AI    | 118 | LYS  |
| 9   | AI    | 121 | ARG  |
| 9   | AI    | 124 | GLN  |
| 10  | AJ    | 13  | HIS  |
| 10  | AJ    | 17  | ASP  |
| 10  | AJ    | 22  | LYS  |
| 10  | AJ    | 25  | GLU  |
| 10  | AJ    | 35  | SER  |
| 10  | AJ    | 40  | LEU  |
| 10  | AJ    | 49  | VAL  |
| 10  | AJ    | 54  | PHE  |
| 10  | AJ    | 55  | LYS  |
| 10  | AJ    | 57  | LYS  |
| 10  | AJ    | 59  | SER  |
| 10  | AJ    | 62  | HIS  |
| 10  | AJ    | 63  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AJ    | 67  | THR  |
| 10  | AJ    | 70  | ARG  |
| 10  | AJ    | 74  | ILE  |
| 10  | AJ    | 80  | LYS  |
| 10  | AJ    | 81  | THR  |
| 10  | AJ    | 90  | LEU  |
| 10  | AJ    | 96  | ILE  |
| 11  | AK    | 18  | ARG  |
| 11  | AK    | 24  | SER  |
| 11  | AK    | 26  | ASN  |
| 11  | AK    | 29  | ILE  |
| 11  | AK    | 30  | VAL  |
| 11  | AK    | 32  | ILE  |
| 11  | AK    | 38  | ASN  |
| 11  | AK    | 40  | ILE  |
| 11  | AK    | 51  | LYS  |
| 11  | AK    | 63  | LEU  |
| 11  | AK    | 92  | GLU  |
| 11  | AK    | 103 | LEU  |
| 11  | AK    | 116 | HIS  |
| 11  | AK    | 117 | ASN  |
| 11  | AK    | 125 | PHE  |
| 11  | AK    | 127 | LYS  |
| 12  | AL    | 10  | LYS  |
| 12  | AL    | 18  | LYS  |
| 12  | AL    | 24  | LEU  |
| 12  | AL    | 30  | ARG  |
| 12  | AL    | 33  | VAL  |
| 12  | AL    | 34  | CYS  |
| 12  | AL    | 35  | THR  |
| 12  | AL    | 40  | VAL  |
| 12  | AL    | 50  | ARG  |
| 12  | AL    | 64  | THR  |
| 12  | AL    | 70  | GLU  |
| 12  | AL    | 73  | ASN  |
| 12  | AL    | 78  | SER  |
| 12  | AL    | 80  | VAL  |
| 12  | AL    | 81  | LEU  |
| 12  | AL    | 86  | ARG  |
| 12  | AL    | 109 | ASP  |
| 13  | AM    | 12  | ASN  |
| 13  | AM    | 47  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | AM    | 48  | LEU  |
| 13  | AM    | 50  | GLU  |
| 13  | AM    | 56  | LEU  |
| 13  | AM    | 58  | GLU  |
| 13  | AM    | 64  | TRP  |
| 13  | AM    | 65  | LYS  |
| 13  | AM    | 67  | GLU  |
| 13  | AM    | 69  | GLU  |
| 13  | AM    | 82  | MET  |
| 13  | AM    | 91  | ARG  |
| 13  | AM    | 93  | ARG  |
| 13  | AM    | 98  | VAL  |
| 13  | AM    | 102 | ARG  |
| 13  | AM    | 104 | ARG  |
| 13  | AM    | 108 | ARG  |
| 13  | AM    | 109 | THR  |
| 13  | AM    | 115 | LYS  |
| 14  | AN    | 12  | ARG  |
| 14  | AN    | 14  | PRO  |
| 14  | AN    | 16  | PHE  |
| 14  | AN    | 25  | VAL  |
| 14  | AN    | 33  | VAL  |
| 14  | AN    | 35  | ARG  |
| 14  | AN    | 41  | ARG  |
| 14  | AN    | 45  | ARG  |
| 14  | AN    | 53  | LEU  |
| 14  | AN    | 60  | SER  |
| 15  | AO    | 10  | LYS  |
| 15  | AO    | 24  | SER  |
| 15  | AO    | 26  | GLU  |
| 15  | AO    | 34  | LEU  |
| 15  | AO    | 35  | ARG  |
| 15  | AO    | 37  | ASN  |
| 15  | AO    | 38  | ARG  |
| 15  | AO    | 39  | LEU  |
| 15  | AO    | 41  | GLU  |
| 15  | AO    | 47  | LYS  |
| 15  | AO    | 49  | ASP  |
| 15  | AO    | 56  | LEU  |
| 15  | AO    | 65  | ARG  |
| 15  | AO    | 71  | GLN  |
| 15  | AO    | 82  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | AO    | 83  | GLU  |
| 16  | AP    | 1   | MET  |
| 16  | AP    | 26  | ARG  |
| 16  | AP    | 27  | LYS  |
| 16  | AP    | 32  | TYR  |
| 16  | AP    | 62  | VAL  |
| 16  | AP    | 65  | GLN  |
| 16  | AP    | 69  | THR  |
| 16  | AP    | 71  | ARG  |
| 16  | AP    | 82  | GLN  |
| 17  | AQ    | 9   | VAL  |
| 17  | AQ    | 11  | VAL  |
| 17  | AQ    | 26  | GLN  |
| 17  | AQ    | 48  | GLU  |
| 17  | AQ    | 50  | LYS  |
| 17  | AQ    | 52  | LYS  |
| 17  | AQ    | 59  | ILE  |
| 17  | AQ    | 60  | ILE  |
| 17  | AQ    | 66  | SER  |
| 17  | AQ    | 77  | VAL  |
| 17  | AQ    | 78  | GLU  |
| 17  | AQ    | 81  | ARG  |
| 17  | AQ    | 94  | ASN  |
| 17  | AQ    | 98  | LEU  |
| 18  | AR    | 25  | THR  |
| 18  | AR    | 31  | LEU  |
| 18  | AR    | 32  | ARG  |
| 18  | AR    | 40  | LEU  |
| 18  | AR    | 53  | ARG  |
| 18  | AR    | 69  | THR  |
| 18  | AR    | 74  | ARG  |
| 18  | AR    | 87  | ARG  |
| 19  | AS    | 4   | SER  |
| 19  | AS    | 5   | LEU  |
| 19  | AS    | 6   | LYS  |
| 19  | AS    | 7   | LYS  |
| 19  | AS    | 13  | ASP  |
| 19  | AS    | 16  | LEU  |
| 19  | AS    | 22  | LEU  |
| 19  | AS    | 27  | GLU  |
| 19  | AS    | 29  | ARG  |
| 19  | AS    | 37  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | AS    | 39  | THR  |
| 19  | AS    | 41  | VAL  |
| 19  | AS    | 44  | MET  |
| 19  | AS    | 49  | ILE  |
| 19  | AS    | 67  | VAL  |
| 19  | AS    | 79  | THR  |
| 20  | AT    | 18  | GLN  |
| 20  | AT    | 19  | SER  |
| 20  | AT    | 26  | ASN  |
| 20  | AT    | 35  | THR  |
| 20  | AT    | 36  | LEU  |
| 20  | AT    | 41  | ILE  |
| 20  | AT    | 64  | ASP  |
| 20  | AT    | 72  | LEU  |
| 20  | AT    | 75  | ASN  |
| 20  | AT    | 82  | SER  |
| 20  | AT    | 84  | LEU  |
| 20  | AT    | 86  | ARG  |
| 20  | AT    | 93  | GLU  |
| 21  | AU    | 8   | THR  |
| 21  | AU    | 12  | LYS  |
| 21  | AU    | 25  | LYS  |
| 29  | BC    | 24  | GLU  |
| 29  | BC    | 36  | LYS  |
| 29  | BC    | 64  | LEU  |
| 29  | BC    | 77  | ILE  |
| 29  | BC    | 94  | VAL  |
| 30  | BD    | 7   | LYS  |
| 30  | BD    | 10  | THR  |
| 30  | BD    | 13  | ARG  |
| 30  | BD    | 14  | ARG  |
| 30  | BD    | 15  | PHE  |
| 30  | BD    | 20  | ASP  |
| 30  | BD    | 21  | PHE  |
| 30  | BD    | 24  | ILE  |
| 30  | BD    | 26  | LYS  |
| 30  | BD    | 36  | PRO  |
| 30  | BD    | 44  | ASN  |
| 30  | BD    | 46  | GLN  |
| 30  | BD    | 48  | ARG  |
| 30  | BD    | 49  | ILE  |
| 30  | BD    | 50  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BD    | 52  | ARG  |
| 30  | BD    | 61  | LEU  |
| 30  | BD    | 65  | ILE  |
| 30  | BD    | 69  | ARG  |
| 30  | BD    | 73  | VAL  |
| 30  | BD    | 75  | ILE  |
| 30  | BD    | 76  | PRO  |
| 30  | BD    | 94  | LEU  |
| 30  | BD    | 106 | ILE  |
| 30  | BD    | 111 | LEU  |
| 30  | BD    | 112 | GLN  |
| 30  | BD    | 113 | VAL  |
| 30  | BD    | 117 | VAL  |
| 30  | BD    | 122 | ASP  |
| 30  | BD    | 127 | VAL  |
| 30  | BD    | 131 | LEU  |
| 30  | BD    | 142 | VAL  |
| 30  | BD    | 146 | GLU  |
| 30  | BD    | 166 | GLN  |
| 30  | BD    | 192 | THR  |
| 30  | BD    | 198 | ASN  |
| 30  | BD    | 201 | HIS  |
| 30  | BD    | 211 | ARG  |
| 30  | BD    | 212 | SER  |
| 30  | BD    | 213 | ARG  |
| 30  | BD    | 218 | ARG  |
| 30  | BD    | 219 | PRO  |
| 30  | BD    | 220 | HIS  |
| 30  | BD    | 221 | VAL  |
| 30  | BD    | 229 | VAL  |
| 30  | BD    | 232 | PRO  |
| 30  | BD    | 252 | TRP  |
| 30  | BD    | 254 | THR  |
| 30  | BD    | 259 | THR  |
| 30  | BD    | 260 | ARG  |
| 30  | BD    | 271 | ILE  |
| 31  | BE    | 7   | VAL  |
| 31  | BE    | 14  | ILE  |
| 31  | BE    | 19  | ARG  |
| 31  | BE    | 24  | THR  |
| 31  | BE    | 33  | VAL  |
| 31  | BE    | 36  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BE    | 40  | GLU  |
| 31  | BE    | 52  | LEU  |
| 31  | BE    | 55  | ASN  |
| 31  | BE    | 61  | ARG  |
| 31  | BE    | 78  | LEU  |
| 31  | BE    | 79  | ARG  |
| 31  | BE    | 82  | ARG  |
| 31  | BE    | 86  | PRO  |
| 31  | BE    | 89  | ASP  |
| 31  | BE    | 92  | THR  |
| 31  | BE    | 94  | GLU  |
| 31  | BE    | 95  | ILE  |
| 31  | BE    | 102 | VAL  |
| 31  | BE    | 107 | THR  |
| 31  | BE    | 113 | PHE  |
| 31  | BE    | 118 | LYS  |
| 31  | BE    | 119 | ARG  |
| 31  | BE    | 134 | ILE  |
| 31  | BE    | 140 | SER  |
| 31  | BE    | 144 | ARG  |
| 31  | BE    | 146 | THR  |
| 31  | BE    | 150 | VAL  |
| 31  | BE    | 154 | LYS  |
| 31  | BE    | 164 | ARG  |
| 31  | BE    | 167 | VAL  |
| 31  | BE    | 173 | VAL  |
| 31  | BE    | 179 | GLU  |
| 31  | BE    | 181 | LEU  |
| 31  | BE    | 189 | PRO  |
| 31  | BE    | 197 | ILE  |
| 31  | BE    | 202 | LYS  |
| 31  | BE    | 203 | LYS  |
| 32  | BF    | 2   | LYS  |
| 32  | BF    | 3   | GLU  |
| 32  | BF    | 20  | LEU  |
| 32  | BF    | 25  | PRO  |
| 32  | BF    | 35  | GLU  |
| 32  | BF    | 38  | ARG  |
| 32  | BF    | 44  | ARG  |
| 32  | BF    | 57  | VAL  |
| 32  | BF    | 67  | GLN  |
| 32  | BF    | 78  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | BF    | 82  | ILE  |
| 32  | BF    | 84  | VAL  |
| 32  | BF    | 88  | VAL  |
| 32  | BF    | 100 | THR  |
| 32  | BF    | 102 | PRO  |
| 32  | BF    | 106 | ARG  |
| 32  | BF    | 107 | LYS  |
| 32  | BF    | 108 | LYS  |
| 32  | BF    | 117 | ARG  |
| 32  | BF    | 125 | LEU  |
| 32  | BF    | 140 | LEU  |
| 32  | BF    | 151 | SER  |
| 32  | BF    | 160 | ASN  |
| 32  | BF    | 164 | ARG  |
| 32  | BF    | 183 | VAL  |
| 32  | BF    | 186 | ILE  |
| 32  | BF    | 194 | MET  |
| 32  | BF    | 202 | PHE  |
| 32  | BF    | 203 | GLN  |
| 33  | BG    | 3   | LEU  |
| 33  | BG    | 4   | ASP  |
| 33  | BG    | 8   | LYS  |
| 33  | BG    | 16  | ARG  |
| 33  | BG    | 21  | ARG  |
| 33  | BG    | 26  | GLN  |
| 33  | BG    | 40  | ASN  |
| 33  | BG    | 52  | ILE  |
| 33  | BG    | 53  | LEU  |
| 33  | BG    | 62  | LEU  |
| 33  | BG    | 63  | ILE  |
| 33  | BG    | 64  | THR  |
| 33  | BG    | 70  | VAL  |
| 33  | BG    | 87  | PRO  |
| 33  | BG    | 88  | ILE  |
| 33  | BG    | 90  | LEU  |
| 33  | BG    | 93  | THR  |
| 33  | BG    | 101 | ILE  |
| 33  | BG    | 103 | LEU  |
| 33  | BG    | 104 | GLU  |
| 33  | BG    | 105 | LYS  |
| 33  | BG    | 111 | LEU  |
| 33  | BG    | 113 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | BG    | 114 | ILE  |
| 33  | BG    | 116 | ASP  |
| 33  | BG    | 123 | ASN  |
| 33  | BG    | 130 | ASN  |
| 33  | BG    | 136 | ARG  |
| 33  | BG    | 139 | LEU  |
| 33  | BG    | 149 | VAL  |
| 33  | BG    | 150 | ASP  |
| 33  | BG    | 153 | ARG  |
| 33  | BG    | 157 | ILE  |
| 33  | BG    | 159 | VAL  |
| 33  | BG    | 161 | THR  |
| 33  | BG    | 162 | THR  |
| 33  | BG    | 170 | ARG  |
| 33  | BG    | 175 | LEU  |
| 34  | BH    | 10  | PRO  |
| 34  | BH    | 12  | PRO  |
| 34  | BH    | 13  | LYS  |
| 34  | BH    | 17  | VAL  |
| 34  | BH    | 21  | PRO  |
| 34  | BH    | 25  | LYS  |
| 34  | BH    | 34  | GLU  |
| 34  | BH    | 41  | MET  |
| 34  | BH    | 46  | GLU  |
| 34  | BH    | 54  | ARG  |
| 34  | BH    | 61  | HIS  |
| 34  | BH    | 68  | THR  |
| 34  | BH    | 76  | VAL  |
| 34  | BH    | 84  | SER  |
| 34  | BH    | 85  | LYS  |
| 34  | BH    | 88  | LEU  |
| 34  | BH    | 103 | LEU  |
| 34  | BH    | 116 | GLU  |
| 34  | BH    | 133 | VAL  |
| 34  | BH    | 139 | GLN  |
| 34  | BH    | 151 | ILE  |
| 34  | BH    | 153 | LYS  |
| 34  | BH    | 157 | TYR  |
| 34  | BH    | 159 | GLU  |
| 34  | BH    | 170 | ARG  |
| 35  | BI    | 7   | GLU  |
| 35  | BI    | 14  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BI    | 23  | PRO  |
| 35  | BI    | 28  | ASN  |
| 35  | BI    | 37  | VAL  |
| 35  | BI    | 38  | LEU  |
| 35  | BI    | 43  | ASN  |
| 35  | BI    | 47  | LEU  |
| 35  | BI    | 60  | GLU  |
| 35  | BI    | 72  | LEU  |
| 35  | BI    | 77  | LEU  |
| 35  | BI    | 82  | ARG  |
| 35  | BI    | 89  | TYR  |
| 35  | BI    | 93  | THR  |
| 35  | BI    | 96  | ASP  |
| 35  | BI    | 99  | GLU  |
| 35  | BI    | 114 | LEU  |
| 35  | BI    | 121 | LYS  |
| 35  | BI    | 122 | GLU  |
| 35  | BI    | 130 | TYR  |
| 35  | BI    | 134 | PRO  |
| 35  | BI    | 138 | ILE  |
| 35  | BI    | 143 | SER  |
| 36  | BN    | 4   | TYR  |
| 36  | BN    | 8   | GLN  |
| 36  | BN    | 9   | VAL  |
| 36  | BN    | 12  | ARG  |
| 36  | BN    | 15  | LEU  |
| 36  | BN    | 17  | ASP  |
| 36  | BN    | 23  | LEU  |
| 36  | BN    | 32  | THR  |
| 36  | BN    | 34  | LEU  |
| 36  | BN    | 38  | HIS  |
| 36  | BN    | 39  | ARG  |
| 36  | BN    | 48  | MET  |
| 36  | BN    | 56  | ASN  |
| 36  | BN    | 60  | ILE  |
| 36  | BN    | 65  | LYS  |
| 36  | BN    | 67  | LEU  |
| 36  | BN    | 68  | GLU  |
| 36  | BN    | 87  | LEU  |
| 36  | BN    | 98  | VAL  |
| 36  | BN    | 99  | LEU  |
| 36  | BN    | 106 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | BN    | 112 | LEU  |
| 36  | BN    | 115 | ARG  |
| 36  | BN    | 120 | LEU  |
| 36  | BN    | 121 | LYS  |
| 36  | BN    | 127 | ASP  |
| 36  | BN    | 134 | ARG  |
| 36  | BN    | 135 | PRO  |
| 36  | BN    | 136 | GLU  |
| 37  | BO    | 1   | MET  |
| 37  | BO    | 2   | ILE  |
| 37  | BO    | 3   | GLN  |
| 37  | BO    | 8   | LEU  |
| 37  | BO    | 14  | THR  |
| 37  | BO    | 17  | ARG  |
| 37  | BO    | 23  | ARG  |
| 37  | BO    | 24  | VAL  |
| 37  | BO    | 25  | LEU  |
| 37  | BO    | 31  | LYS  |
| 37  | BO    | 32  | TYR  |
| 37  | BO    | 48  | PRO  |
| 37  | BO    | 52  | VAL  |
| 37  | BO    | 68  | GLU  |
| 37  | BO    | 73  | ASP  |
| 37  | BO    | 78  | ARG  |
| 37  | BO    | 92  | GLU  |
| 37  | BO    | 99  | PHE  |
| 37  | BO    | 117 | LEU  |
| 38  | BP    | 9   | ASN  |
| 38  | BP    | 10  | PRO  |
| 38  | BP    | 13  | ASN  |
| 38  | BP    | 15  | ARG  |
| 38  | BP    | 16  | ARG  |
| 38  | BP    | 19  | VAL  |
| 38  | BP    | 21  | ARG  |
| 38  | BP    | 32  | THR  |
| 38  | BP    | 38  | GLN  |
| 38  | BP    | 39  | LYS  |
| 38  | BP    | 41  | ARG  |
| 38  | BP    | 42  | SER  |
| 38  | BP    | 45  | LEU  |
| 38  | BP    | 49  | ARG  |
| 38  | BP    | 59  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BP    | 61  | ARG  |
| 38  | BP    | 63  | PRO  |
| 38  | BP    | 64  | LYS  |
| 38  | BP    | 65  | ARG  |
| 38  | BP    | 67  | MET  |
| 38  | BP    | 68  | GLN  |
| 38  | BP    | 83  | VAL  |
| 38  | BP    | 85  | LEU  |
| 38  | BP    | 88  | LEU  |
| 38  | BP    | 91  | PHE  |
| 38  | BP    | 98  | GLU  |
| 38  | BP    | 100 | LEU  |
| 38  | BP    | 105 | LEU  |
| 38  | BP    | 108 | LYS  |
| 38  | BP    | 110 | TYR  |
| 38  | BP    | 114 | ILE  |
| 38  | BP    | 117 | GLU  |
| 38  | BP    | 119 | GLU  |
| 38  | BP    | 123 | LEU  |
| 38  | BP    | 130 | PHE  |
| 38  | BP    | 132 | LYS  |
| 39  | BQ    | 1   | MET  |
| 39  | BQ    | 5   | ARG  |
| 39  | BQ    | 6   | ARG  |
| 39  | BQ    | 11  | LYS  |
| 39  | BQ    | 13  | GLN  |
| 39  | BQ    | 21  | THR  |
| 39  | BQ    | 25  | ASP  |
| 39  | BQ    | 51  | ARG  |
| 39  | BQ    | 52  | VAL  |
| 39  | BQ    | 55  | VAL  |
| 39  | BQ    | 58  | PHE  |
| 39  | BQ    | 76  | LYS  |
| 39  | BQ    | 81  | VAL  |
| 39  | BQ    | 103 | MET  |
| 39  | BQ    | 110 | THR  |
| 39  | BQ    | 111 | GLU  |
| 39  | BQ    | 112 | GLU  |
| 39  | BQ    | 113 | GLN  |
| 39  | BQ    | 115 | MET  |
| 39  | BQ    | 116 | GLU  |
| 39  | BQ    | 125 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BQ    | 133 | ARG  |
| 39  | BQ    | 134 | ARG  |
| 39  | BQ    | 135 | ASP  |
| 39  | BQ    | 137 | TYR  |
| 39  | BQ    | 139 | GLU  |
| 40  | BR    | 2   | ARG  |
| 40  | BR    | 4   | LEU  |
| 40  | BR    | 5   | LYS  |
| 40  | BR    | 6   | SER  |
| 40  | BR    | 8   | ARG  |
| 40  | BR    | 14  | SER  |
| 40  | BR    | 16  | HIS  |
| 40  | BR    | 18  | LEU  |
| 40  | BR    | 27  | SER  |
| 40  | BR    | 35  | THR  |
| 40  | BR    | 48  | VAL  |
| 40  | BR    | 49  | ASP  |
| 40  | BR    | 51  | LEU  |
| 40  | BR    | 54  | LEU  |
| 40  | BR    | 56  | LYS  |
| 40  | BR    | 60  | LEU  |
| 40  | BR    | 67  | LEU  |
| 40  | BR    | 71  | GLN  |
| 40  | BR    | 75  | LEU  |
| 40  | BR    | 76  | VAL  |
| 40  | BR    | 79  | LEU  |
| 40  | BR    | 81  | ASP  |
| 40  | BR    | 103 | ARG  |
| 41  | BS    | 11  | LYS  |
| 41  | BS    | 18  | ILE  |
| 41  | BS    | 20  | ARG  |
| 41  | BS    | 21  | THR  |
| 41  | BS    | 24  | LEU  |
| 41  | BS    | 26  | LEU  |
| 41  | BS    | 42  | ASP  |
| 41  | BS    | 65  | VAL  |
| 41  | BS    | 82  | ILE  |
| 41  | BS    | 85  | VAL  |
| 41  | BS    | 89  | ARG  |
| 41  | BS    | 92  | TYR  |
| 41  | BS    | 97  | ARG  |
| 41  | BS    | 99  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BS    | 101 | LEU  |
| 41  | BS    | 103 | GLU  |
| 41  | BS    | 106 | ARG  |
| 42  | BT    | 3   | ARG  |
| 42  | BT    | 6   | LEU  |
| 42  | BT    | 11  | GLU  |
| 42  | BT    | 13  | ARG  |
| 42  | BT    | 14  | TYR  |
| 42  | BT    | 16  | ARG  |
| 42  | BT    | 17  | THR  |
| 42  | BT    | 29  | ARG  |
| 42  | BT    | 31  | SER  |
| 42  | BT    | 32  | TYR  |
| 42  | BT    | 41  | ARG  |
| 42  | BT    | 44  | ASP  |
| 42  | BT    | 49  | VAL  |
| 42  | BT    | 51  | ARG  |
| 42  | BT    | 53  | ARG  |
| 42  | BT    | 59  | THR  |
| 42  | BT    | 62  | THR  |
| 42  | BT    | 65  | LYS  |
| 42  | BT    | 66  | VAL  |
| 42  | BT    | 68  | TYR  |
| 42  | BT    | 74  | ARG  |
| 42  | BT    | 78  | LEU  |
| 42  | BT    | 82  | LEU  |
| 42  | BT    | 84  | GLN  |
| 42  | BT    | 85  | LYS  |
| 42  | BT    | 90  | GLN  |
| 42  | BT    | 91  | ARG  |
| 42  | BT    | 106 | SER  |
| 42  | BT    | 107 | ASP  |
| 42  | BT    | 108 | ARG  |
| 42  | BT    | 110 | ILE  |
| 42  | BT    | 111 | ARG  |
| 42  | BT    | 114 | LEU  |
| 42  | BT    | 121 | ILE  |
| 42  | BT    | 122 | ASP  |
| 42  | BT    | 124 | ASP  |
| 42  | BT    | 125 | ARG  |
| 42  | BT    | 128 | GLU  |
| 42  | BT    | 132 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | BU    | 5   | LYS  |
| 43  | BU    | 9   | VAL  |
| 43  | BU    | 15  | LYS  |
| 43  | BU    | 16  | LYS  |
| 43  | BU    | 19  | LYS  |
| 43  | BU    | 20  | LEU  |
| 43  | BU    | 27  | LEU  |
| 43  | BU    | 31  | SER  |
| 43  | BU    | 33  | ARG  |
| 43  | BU    | 49  | HIS  |
| 43  | BU    | 52  | ARG  |
| 43  | BU    | 60  | LEU  |
| 43  | BU    | 69  | CYS  |
| 43  | BU    | 70  | ARG  |
| 43  | BU    | 72  | HIS  |
| 43  | BU    | 74  | LEU  |
| 43  | BU    | 78  | THR  |
| 43  | BU    | 89  | GLU  |
| 43  | BU    | 92  | ARG  |
| 43  | BU    | 97  | ASP  |
| 43  | BU    | 104 | GLN  |
| 44  | BV    | 2   | PHE  |
| 44  | BV    | 14  | VAL  |
| 44  | BV    | 16  | PRO  |
| 44  | BV    | 18  | LEU  |
| 44  | BV    | 19  | LYS  |
| 44  | BV    | 35  | LEU  |
| 44  | BV    | 37  | VAL  |
| 44  | BV    | 39  | LEU  |
| 44  | BV    | 43  | GLU  |
| 44  | BV    | 49  | THR  |
| 44  | BV    | 52  | VAL  |
| 44  | BV    | 62  | LEU  |
| 44  | BV    | 64  | HIS  |
| 44  | BV    | 66  | ARG  |
| 44  | BV    | 69  | LYS  |
| 44  | BV    | 79  | VAL  |
| 44  | BV    | 82  | ARG  |
| 44  | BV    | 88  | ARG  |
| 44  | BV    | 91  | TYR  |
| 44  | BV    | 92  | THR  |
| 44  | BV    | 95  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | BV    | 99  | ILE  |
| 44  | BV    | 100 | ARG  |
| 45  | BW    | 6   | ILE  |
| 45  | BW    | 11  | ARG  |
| 45  | BW    | 13  | SER  |
| 45  | BW    | 19  | LEU  |
| 45  | BW    | 33  | ARG  |
| 45  | BW    | 34  | ASN  |
| 45  | BW    | 36  | LEU  |
| 45  | BW    | 39  | THR  |
| 45  | BW    | 51  | LEU  |
| 45  | BW    | 60  | ASN  |
| 45  | BW    | 66  | GLU  |
| 45  | BW    | 67  | ASP  |
| 45  | BW    | 83  | LYS  |
| 45  | BW    | 90  | ARG  |
| 45  | BW    | 92  | ARG  |
| 45  | BW    | 106 | ILE  |
| 45  | BW    | 107 | LEU  |
| 46  | BX    | 11  | PRO  |
| 46  | BX    | 13  | LEU  |
| 46  | BX    | 27  | THR  |
| 46  | BX    | 28  | PHE  |
| 46  | BX    | 30  | VAL  |
| 46  | BX    | 38  | GLU  |
| 46  | BX    | 48  | LYS  |
| 46  | BX    | 57  | LEU  |
| 46  | BX    | 66  | LEU  |
| 46  | BX    | 68  | ARG  |
| 46  | BX    | 70  | LEU  |
| 46  | BX    | 76  | ARG  |
| 46  | BX    | 80  | ILE  |
| 46  | BX    | 81  | VAL  |
| 47  | BY    | 2   | ARG  |
| 47  | BY    | 6   | HIS  |
| 47  | BY    | 7   | VAL  |
| 47  | BY    | 8   | LYS  |
| 47  | BY    | 21  | LYS  |
| 47  | BY    | 28  | LYS  |
| 47  | BY    | 29  | GLU  |
| 47  | BY    | 32  | PRO  |
| 47  | BY    | 47  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | BY    | 53  | PRO  |
| 47  | BY    | 56  | PRO  |
| 47  | BY    | 62  | GLU  |
| 47  | BY    | 66  | PRO  |
| 47  | BY    | 67  | LEU  |
| 47  | BY    | 70  | SER  |
| 47  | BY    | 73  | ARG  |
| 47  | BY    | 76  | CYS  |
| 47  | BY    | 77  | PRO  |
| 47  | BY    | 79  | CYS  |
| 47  | BY    | 89  | PHE  |
| 47  | BY    | 90  | LEU  |
| 47  | BY    | 97  | ARG  |
| 48  | BZ    | 5   | LYS  |
| 48  | BZ    | 22  | LYS  |
| 48  | BZ    | 30  | ARG  |
| 48  | BZ    | 38  | VAL  |
| 48  | BZ    | 40  | LEU  |
| 48  | BZ    | 49  | GLN  |
| 48  | BZ    | 52  | ILE  |
| 48  | BZ    | 66  | LEU  |
| 48  | BZ    | 71  | ARG  |
| 48  | BZ    | 75  | LEU  |
| 48  | BZ    | 78  | ARG  |
| 48  | BZ    | 79  | ARG  |
| 48  | BZ    | 80  | ARG  |
| 48  | BZ    | 81  | ARG  |
| 48  | BZ    | 85  | VAL  |
| 48  | BZ    | 88  | PHE  |
| 48  | BZ    | 101 | LEU  |
| 48  | BZ    | 103 | PHE  |
| 48  | BZ    | 123 | ILE  |
| 48  | BZ    | 131 | ASN  |
| 48  | BZ    | 137 | GLU  |
| 48  | BZ    | 144 | GLU  |
| 48  | BZ    | 147 | ASP  |
| 48  | BZ    | 149 | LEU  |
| 48  | BZ    | 153 | ASP  |
| 48  | BZ    | 154 | LEU  |
| 48  | BZ    | 167 | GLU  |
| 48  | BZ    | 170 | ILE  |
| 49  | B0    | 7   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | B0    | 12  | ASN  |
| 49  | B0    | 14  | ARG  |
| 49  | B0    | 30  | VAL  |
| 49  | B0    | 36  | ILE  |
| 49  | B0    | 37  | LEU  |
| 49  | B0    | 40  | GLN  |
| 49  | B0    | 41  | ARG  |
| 49  | B0    | 53  | MET  |
| 49  | B0    | 55  | ARG  |
| 49  | B0    | 69  | PHE  |
| 49  | B0    | 75  | LEU  |
| 49  | B0    | 84  | LEU  |
| 50  | B1    | 5   | CYS  |
| 50  | B1    | 14  | VAL  |
| 50  | B1    | 16  | ASN  |
| 50  | B1    | 18  | ILE  |
| 50  | B1    | 30  | VAL  |
| 50  | B1    | 35  | THR  |
| 50  | B1    | 40  | ARG  |
| 50  | B1    | 41  | ARG  |
| 50  | B1    | 45  | ASN  |
| 50  | B1    | 46  | LEU  |
| 50  | B1    | 48  | LYS  |
| 50  | B1    | 58  | ILE  |
| 50  | B1    | 61  | ARG  |
| 50  | B1    | 65  | SER  |
| 50  | B1    | 72  | GLU  |
| 50  | B1    | 83  | GLU  |
| 50  | B1    | 94  | LEU  |
| 50  | B1    | 95  | LEU  |
| 51  | B2    | 7   | ARG  |
| 51  | B2    | 9   | GLN  |
| 51  | B2    | 14  | ARG  |
| 51  | B2    | 16  | LEU  |
| 51  | B2    | 17  | SER  |
| 51  | B2    | 30  | ARG  |
| 51  | B2    | 32  | LEU  |
| 51  | B2    | 35  | LEU  |
| 51  | B2    | 43  | GLN  |
| 51  | B2    | 44  | LEU  |
| 51  | B2    | 48  | HIS  |
| 51  | B2    | 52  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | B2    | 53  | LEU  |
| 51  | B2    | 62  | THR  |
| 51  | B2    | 64  | LEU  |
| 51  | B2    | 71  | ASN  |
| 52  | B3    | 6   | VAL  |
| 52  | B3    | 8   | LEU  |
| 52  | B3    | 17  | LYS  |
| 52  | B3    | 18  | ASP  |
| 52  | B3    | 23  | LEU  |
| 52  | B3    | 24  | LYS  |
| 52  | B3    | 30  | ARG  |
| 52  | B3    | 35  | ARG  |
| 52  | B3    | 37  | LEU  |
| 53  | B4    | 44  | CYS  |
| 53  | B4    | 46  | ASN  |
| 53  | B4    | 51  | TYR  |
| 53  | B4    | 56  | GLU  |
| 54  | B5    | 3   | LYS  |
| 54  | B5    | 4   | HIS  |
| 54  | B5    | 6   | VAL  |
| 54  | B5    | 16  | ARG  |
| 54  | B5    | 29  | THR  |
| 54  | B5    | 30  | LEU  |
| 54  | B5    | 32  | PRO  |
| 54  | B5    | 40  | LYS  |
| 54  | B5    | 52  | TYR  |
| 54  | B5    | 56  | LYS  |
| 54  | B5    | 57  | VAL  |
| 54  | B5    | 60  | VAL  |
| 55  | B6    | 9   | LEU  |
| 55  | B6    | 10  | LEU  |
| 55  | B6    | 11  | LEU  |
| 55  | B6    | 17  | LYS  |
| 55  | B6    | 18  | ARG  |
| 55  | B6    | 19  | ARG  |
| 55  | B6    | 20  | ASN  |
| 55  | B6    | 36  | LEU  |
| 55  | B6    | 42  | TRP  |
| 55  | B6    | 47  | THR  |
| 55  | B6    | 48  | VAL  |
| 55  | B6    | 49  | HIS  |
| 55  | B6    | 51  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | B7    | 1   | MET  |
| 56  | B7    | 4   | THR  |
| 56  | B7    | 8   | ASN  |
| 56  | B7    | 9   | ARG  |
| 56  | B7    | 10  | ARG  |
| 56  | B7    | 16  | HIS  |
| 56  | B7    | 24  | THR  |
| 57  | B8    | 8   | LYS  |
| 57  | B8    | 13  | ARG  |
| 57  | B8    | 30  | ARG  |
| 57  | B8    | 31  | HIS  |
| 57  | B8    | 33  | ASN  |
| 57  | B8    | 34  | TRP  |
| 57  | B8    | 35  | GLN  |
| 57  | B8    | 44  | LYS  |
| 57  | B8    | 61  | LEU  |
| 58  | B9    | 2   | LYS  |
| 58  | B9    | 11  | CYS  |
| 58  | B9    | 17  | ILE  |
| 58  | B9    | 20  | HIS  |
| 58  | B9    | 23  | VAL  |
| 58  | B9    | 27  | CYS  |
| 58  | B9    | 28  | GLU  |
| 58  | B9    | 29  | ASN  |
| 58  | B9    | 34  | GLN  |
| 2   | CB    | 15  | VAL  |
| 2   | CB    | 16  | HIS  |
| 2   | CB    | 17  | PHE  |
| 2   | CB    | 20  | GLU  |
| 2   | CB    | 36  | ARG  |
| 2   | CB    | 44  | LEU  |
| 2   | CB    | 69  | LEU  |
| 2   | CB    | 73  | THR  |
| 2   | CB    | 74  | LYS  |
| 2   | CB    | 80  | ILE  |
| 2   | CB    | 90  | MET  |
| 2   | CB    | 92  | TYR  |
| 2   | CB    | 110 | GLN  |
| 2   | CB    | 111 | ARG  |
| 2   | CB    | 112 | VAL  |
| 2   | CB    | 115 | LEU  |
| 2   | CB    | 137 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 145 | LEU  |
| 2   | CB    | 155 | LEU  |
| 2   | CB    | 158 | LEU  |
| 2   | CB    | 172 | ILE  |
| 2   | CB    | 187 | LEU  |
| 2   | CB    | 190 | THR  |
| 2   | CB    | 196 | LEU  |
| 2   | CB    | 198 | ASP  |
| 2   | CB    | 210 | SER  |
| 2   | CB    | 233 | SER  |
| 2   | CB    | 238 | LEU  |
| 3   | CC    | 12  | LEU  |
| 3   | CC    | 20  | SER  |
| 3   | CC    | 21  | ARG  |
| 3   | CC    | 29  | TYR  |
| 3   | CC    | 30  | ARG  |
| 3   | CC    | 34  | LEU  |
| 3   | CC    | 42  | LEU  |
| 3   | CC    | 52  | LEU  |
| 3   | CC    | 55  | VAL  |
| 3   | CC    | 94  | LEU  |
| 3   | CC    | 104 | GLN  |
| 3   | CC    | 127 | ARG  |
| 3   | CC    | 128 | PHE  |
| 3   | CC    | 131 | ARG  |
| 3   | CC    | 156 | ARG  |
| 3   | CC    | 165 | THR  |
| 3   | CC    | 188 | LEU  |
| 3   | CC    | 193 | TYR  |
| 3   | CC    | 196 | LEU  |
| 3   | CC    | 202 | ILE  |
| 4   | CD    | 3   | ARG  |
| 4   | CD    | 7   | PRO  |
| 4   | CD    | 9   | CYS  |
| 4   | CD    | 10  | ARG  |
| 4   | CD    | 11  | LEU  |
| 4   | CD    | 24  | GLU  |
| 4   | CD    | 26  | CYS  |
| 4   | CD    | 28  | SER  |
| 4   | CD    | 31  | CYS  |
| 4   | CD    | 33  | MET  |
| 4   | CD    | 49  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CD    | 53  | ASP  |
| 4   | CD    | 78  | LEU  |
| 4   | CD    | 96  | LEU  |
| 4   | CD    | 119 | GLN  |
| 4   | CD    | 120 | LEU  |
| 4   | CD    | 131 | ARG  |
| 4   | CD    | 135 | LEU  |
| 4   | CD    | 138 | TYR  |
| 4   | CD    | 140 | VAL  |
| 4   | CD    | 144 | ASP  |
| 4   | CD    | 146 | ILE  |
| 4   | CD    | 153 | ARG  |
| 4   | CD    | 163 | GLU  |
| 4   | CD    | 173 | TRP  |
| 4   | CD    | 175 | SER  |
| 4   | CD    | 177 | ASP  |
| 4   | CD    | 182 | LYS  |
| 4   | CD    | 185 | PHE  |
| 4   | CD    | 192 | GLU  |
| 4   | CD    | 193 | ASP  |
| 4   | CD    | 194 | LEU  |
| 4   | CD    | 204 | ILE  |
| 5   | CE    | 10  | MET  |
| 5   | CE    | 20  | GLN  |
| 5   | CE    | 41  | VAL  |
| 5   | CE    | 45  | PHE  |
| 5   | CE    | 64  | ARG  |
| 5   | CE    | 68  | GLU  |
| 5   | CE    | 73  | ASN  |
| 5   | CE    | 76  | ILE  |
| 5   | CE    | 79  | GLU  |
| 5   | CE    | 80  | ILE  |
| 5   | CE    | 87  | SER  |
| 5   | CE    | 101 | ILE  |
| 5   | CE    | 115 | VAL  |
| 5   | CE    | 116 | THR  |
| 5   | CE    | 125 | SER  |
| 5   | CE    | 126 | ARG  |
| 5   | CE    | 128 | PRO  |
| 5   | CE    | 147 | ASP  |
| 5   | CE    | 148 | VAL  |
| 6   | CF    | 10  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | CF    | 16  | GLN  |
| 6   | CF    | 19  | LEU  |
| 6   | CF    | 21  | LEU  |
| 6   | CF    | 27  | GLN  |
| 6   | CF    | 69  | GLU  |
| 6   | CF    | 73  | ASN  |
| 6   | CF    | 80  | ARG  |
| 6   | CF    | 83  | ASP  |
| 6   | CF    | 90  | VAL  |
| 6   | CF    | 93  | SER  |
| 6   | CF    | 100 | ASN  |
| 7   | CG    | 4   | ARG  |
| 7   | CG    | 12  | LEU  |
| 7   | CG    | 17  | VAL  |
| 7   | CG    | 24  | THR  |
| 7   | CG    | 30  | ILE  |
| 7   | CG    | 32  | ARG  |
| 7   | CG    | 38  | LEU  |
| 7   | CG    | 45  | ASP  |
| 7   | CG    | 52  | GLU  |
| 7   | CG    | 58  | PRO  |
| 7   | CG    | 60  | LYS  |
| 7   | CG    | 77  | SER  |
| 7   | CG    | 79  | ARG  |
| 7   | CG    | 84  | ASN  |
| 7   | CG    | 88  | PRO  |
| 7   | CG    | 92  | SER  |
| 7   | CG    | 114 | ARG  |
| 7   | CG    | 124 | LEU  |
| 7   | CG    | 131 | LYS  |
| 7   | CG    | 142 | GLU  |
| 8   | CH    | 1   | MET  |
| 8   | CH    | 4   | ASP  |
| 8   | CH    | 8   | ASP  |
| 8   | CH    | 10  | LEU  |
| 8   | CH    | 52  | ASP  |
| 8   | CH    | 63  | LEU  |
| 8   | CH    | 65  | TYR  |
| 8   | CH    | 85  | ARG  |
| 8   | CH    | 102 | ARG  |
| 8   | CH    | 104 | ARG  |
| 8   | CH    | 105 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | CH    | 119 | LEU  |
| 8   | CH    | 127 | LEU  |
| 8   | CH    | 129 | VAL  |
| 9   | CI    | 10  | ARG  |
| 9   | CI    | 40  | LEU  |
| 9   | CI    | 53  | VAL  |
| 9   | CI    | 95  | LYS  |
| 9   | CI    | 99  | LEU  |
| 9   | CI    | 103 | THR  |
| 9   | CI    | 104 | ARG  |
| 9   | CI    | 112 | LYS  |
| 9   | CI    | 114 | TYR  |
| 9   | CI    | 121 | ARG  |
| 9   | CI    | 125 | TYR  |
| 9   | CI    | 128 | ARG  |
| 10  | CJ    | 6   | ILE  |
| 10  | CJ    | 16  | LEU  |
| 10  | CJ    | 22  | LYS  |
| 10  | CJ    | 40  | LEU  |
| 10  | CJ    | 45  | ARG  |
| 10  | CJ    | 47  | PHE  |
| 10  | CJ    | 50  | ILE  |
| 10  | CJ    | 62  | HIS  |
| 10  | CJ    | 63  | PHE  |
| 10  | CJ    | 67  | THR  |
| 10  | CJ    | 80  | LYS  |
| 10  | CJ    | 86  | MET  |
| 10  | CJ    | 92  | THR  |
| 10  | CJ    | 96  | ILE  |
| 11  | CK    | 18  | ARG  |
| 11  | CK    | 33  | THR  |
| 11  | CK    | 50  | TYR  |
| 11  | CK    | 51  | LYS  |
| 11  | CK    | 87  | THR  |
| 11  | CK    | 103 | LEU  |
| 11  | CK    | 109 | VAL  |
| 11  | CK    | 114 | VAL  |
| 11  | CK    | 119 | CYS  |
| 11  | CK    | 124 | LYS  |
| 11  | CK    | 125 | PHE  |
| 11  | CK    | 129 | SER  |
| 12  | CL    | 18  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | CL    | 24  | LEU  |
| 12  | CL    | 30  | ARG  |
| 12  | CL    | 39  | THR  |
| 12  | CL    | 41  | THR  |
| 12  | CL    | 50  | ARG  |
| 12  | CL    | 66  | TYR  |
| 12  | CL    | 70  | GLU  |
| 12  | CL    | 73  | ASN  |
| 12  | CL    | 77  | HIS  |
| 12  | CL    | 81  | LEU  |
| 12  | CL    | 86  | ARG  |
| 12  | CL    | 89  | ASP  |
| 12  | CL    | 124 | GLU  |
| 13  | CM    | 12  | ASN  |
| 13  | CM    | 14  | ARG  |
| 13  | CM    | 32  | GLU  |
| 13  | CM    | 47  | ASP  |
| 13  | CM    | 48  | LEU  |
| 13  | CM    | 50  | GLU  |
| 13  | CM    | 64  | TRP  |
| 13  | CM    | 65  | LYS  |
| 13  | CM    | 66  | LEU  |
| 13  | CM    | 67  | GLU  |
| 13  | CM    | 69  | GLU  |
| 13  | CM    | 70  | LEU  |
| 13  | CM    | 71  | ARG  |
| 13  | CM    | 82  | MET  |
| 13  | CM    | 84  | ILE  |
| 13  | CM    | 92  | HIS  |
| 13  | CM    | 93  | ARG  |
| 13  | CM    | 98  | VAL  |
| 13  | CM    | 110 | ARG  |
| 14  | CN    | 8   | GLU  |
| 14  | CN    | 12  | ARG  |
| 14  | CN    | 14  | PRO  |
| 14  | CN    | 18  | VAL  |
| 14  | CN    | 23  | ARG  |
| 14  | CN    | 26  | ARG  |
| 14  | CN    | 27  | CYS  |
| 14  | CN    | 33  | VAL  |
| 14  | CN    | 34  | TYR  |
| 14  | CN    | 35  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | CN    | 42  | ILE  |
| 14  | CN    | 44  | LEU  |
| 15  | CO    | 3   | ILE  |
| 15  | CO    | 10  | LYS  |
| 15  | CO    | 22  | THR  |
| 15  | CO    | 37  | ASN  |
| 15  | CO    | 39  | LEU  |
| 15  | CO    | 47  | LYS  |
| 15  | CO    | 51  | HIS  |
| 15  | CO    | 54  | ARG  |
| 15  | CO    | 62  | GLN  |
| 15  | CO    | 65  | ARG  |
| 15  | CO    | 66  | LEU  |
| 15  | CO    | 71  | GLN  |
| 15  | CO    | 82  | ILE  |
| 15  | CO    | 83  | GLU  |
| 16  | CP    | 1   | MET  |
| 16  | CP    | 11  | SER  |
| 16  | CP    | 12  | LYS  |
| 16  | CP    | 16  | HIS  |
| 16  | CP    | 26  | ARG  |
| 16  | CP    | 27  | LYS  |
| 16  | CP    | 53  | VAL  |
| 16  | CP    | 61  | SER  |
| 16  | CP    | 65  | GLN  |
| 16  | CP    | 67  | THR  |
| 16  | CP    | 69  | THR  |
| 16  | CP    | 82  | GLN  |
| 17  | CQ    | 5   | VAL  |
| 17  | CQ    | 9   | VAL  |
| 17  | CQ    | 10  | VAL  |
| 17  | CQ    | 14  | LYS  |
| 17  | CQ    | 23  | VAL  |
| 17  | CQ    | 52  | LYS  |
| 17  | CQ    | 56  | VAL  |
| 17  | CQ    | 83  | ASP  |
| 17  | CQ    | 89  | LEU  |
| 17  | CQ    | 97  | SER  |
| 18  | CR    | 19  | LYS  |
| 18  | CR    | 26  | LEU  |
| 18  | CR    | 36  | ASN  |
| 18  | CR    | 38  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | CR    | 69  | THR  |
| 18  | CR    | 87  | ARG  |
| 19  | CS    | 5   | LEU  |
| 19  | CS    | 6   | LYS  |
| 19  | CS    | 7   | LYS  |
| 19  | CS    | 11  | VAL  |
| 19  | CS    | 13  | ASP  |
| 19  | CS    | 22  | LEU  |
| 19  | CS    | 23  | ASN  |
| 19  | CS    | 27  | GLU  |
| 19  | CS    | 28  | LYS  |
| 19  | CS    | 29  | ARG  |
| 19  | CS    | 32  | LYS  |
| 19  | CS    | 37  | ARG  |
| 19  | CS    | 43  | GLU  |
| 19  | CS    | 44  | MET  |
| 19  | CS    | 49  | ILE  |
| 19  | CS    | 64  | GLU  |
| 19  | CS    | 65  | ASN  |
| 19  | CS    | 79  | THR  |
| 20  | CT    | 14  | LYS  |
| 20  | CT    | 26  | ASN  |
| 20  | CT    | 36  | LEU  |
| 20  | CT    | 41  | ILE  |
| 20  | CT    | 62  | LEU  |
| 20  | CT    | 64  | ASP  |
| 20  | CT    | 75  | ASN  |
| 20  | CT    | 82  | SER  |
| 20  | CT    | 90  | GLN  |
| 20  | CT    | 93  | GLU  |
| 20  | CT    | 104 | LEU  |
| 21  | CU    | 12  | LYS  |
| 29  | DC    | 20  | TYR  |
| 29  | DC    | 24  | GLU  |
| 29  | DC    | 36  | LYS  |
| 29  | DC    | 47  | LEU  |
| 29  | DC    | 55  | ASP  |
| 29  | DC    | 56  | GLN  |
| 29  | DC    | 58  | VAL  |
| 29  | DC    | 64  | LEU  |
| 29  | DC    | 77  | ILE  |
| 29  | DC    | 93  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DD    | 10  | THR  |
| 30  | DD    | 13  | ARG  |
| 30  | DD    | 18  | VAL  |
| 30  | DD    | 20  | ASP  |
| 30  | DD    | 26  | LYS  |
| 30  | DD    | 29  | PRO  |
| 30  | DD    | 37  | LEU  |
| 30  | DD    | 43  | ARG  |
| 30  | DD    | 58  | HIS  |
| 30  | DD    | 61  | LEU  |
| 30  | DD    | 65  | ILE  |
| 30  | DD    | 73  | VAL  |
| 30  | DD    | 86  | PRO  |
| 30  | DD    | 92  | ILE  |
| 30  | DD    | 94  | LEU  |
| 30  | DD    | 98  | VAL  |
| 30  | DD    | 104 | TYR  |
| 30  | DD    | 105 | ILE  |
| 30  | DD    | 140 | THR  |
| 30  | DD    | 147 | LEU  |
| 30  | DD    | 154 | LYS  |
| 30  | DD    | 155 | LEU  |
| 30  | DD    | 165 | ILE  |
| 30  | DD    | 168 | ARG  |
| 30  | DD    | 173 | VAL  |
| 30  | DD    | 178 | PRO  |
| 30  | DD    | 192 | THR  |
| 30  | DD    | 202 | LYS  |
| 30  | DD    | 204 | ILE  |
| 30  | DD    | 208 | LYS  |
| 30  | DD    | 218 | ARG  |
| 30  | DD    | 228 | PRO  |
| 30  | DD    | 230 | ASP  |
| 30  | DD    | 231 | HIS  |
| 30  | DD    | 239 | ARG  |
| 30  | DD    | 242 | ARG  |
| 30  | DD    | 246 | PRO  |
| 30  | DD    | 254 | THR  |
| 30  | DD    | 259 | THR  |
| 30  | DD    | 260 | ARG  |
| 31  | DE    | 1   | MET  |
| 31  | DE    | 4   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | DE    | 7   | VAL  |
| 31  | DE    | 9   | VAL  |
| 31  | DE    | 16  | ARG  |
| 31  | DE    | 18  | ASP  |
| 31  | DE    | 22  | PRO  |
| 31  | DE    | 23  | VAL  |
| 31  | DE    | 24  | THR  |
| 31  | DE    | 30  | PRO  |
| 31  | DE    | 40  | GLU  |
| 31  | DE    | 52  | LEU  |
| 31  | DE    | 55  | ASN  |
| 31  | DE    | 57  | LYS  |
| 31  | DE    | 76  | ARG  |
| 31  | DE    | 78  | LEU  |
| 31  | DE    | 79  | ARG  |
| 31  | DE    | 82  | ARG  |
| 31  | DE    | 84  | PHE  |
| 31  | DE    | 86  | PRO  |
| 31  | DE    | 89  | ASP  |
| 31  | DE    | 92  | THR  |
| 31  | DE    | 101 | ARG  |
| 31  | DE    | 105 | THR  |
| 31  | DE    | 107 | THR  |
| 31  | DE    | 113 | PHE  |
| 31  | DE    | 116 | VAL  |
| 31  | DE    | 118 | LYS  |
| 31  | DE    | 119 | ARG  |
| 31  | DE    | 121 | ASN  |
| 31  | DE    | 127 | ASP  |
| 31  | DE    | 128 | SER  |
| 31  | DE    | 134 | ILE  |
| 31  | DE    | 144 | ARG  |
| 31  | DE    | 150 | VAL  |
| 31  | DE    | 154 | LYS  |
| 31  | DE    | 159 | HIS  |
| 31  | DE    | 166 | THR  |
| 31  | DE    | 168 | MET  |
| 31  | DE    | 179 | GLU  |
| 31  | DE    | 185 | LYS  |
| 31  | DE    | 197 | ILE  |
| 31  | DE    | 202 | LYS  |
| 31  | DE    | 203 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | DF    | 2   | LYS  |
| 32  | DF    | 4   | VAL  |
| 32  | DF    | 25  | PRO  |
| 32  | DF    | 28  | ILE  |
| 32  | DF    | 38  | ARG  |
| 32  | DF    | 46  | ARG  |
| 32  | DF    | 53  | THR  |
| 32  | DF    | 65  | TRP  |
| 32  | DF    | 66  | PRO  |
| 32  | DF    | 67  | GLN  |
| 32  | DF    | 78  | ILE  |
| 32  | DF    | 81  | PRO  |
| 32  | DF    | 88  | VAL  |
| 32  | DF    | 99  | TYR  |
| 32  | DF    | 100 | THR  |
| 32  | DF    | 102 | PRO  |
| 32  | DF    | 112 | MET  |
| 32  | DF    | 125 | LEU  |
| 32  | DF    | 136 | THR  |
| 32  | DF    | 149 | ASP  |
| 32  | DF    | 158 | THR  |
| 32  | DF    | 175 | THR  |
| 32  | DF    | 183 | VAL  |
| 32  | DF    | 186 | ILE  |
| 32  | DF    | 190 | GLU  |
| 32  | DF    | 195 | ASP  |
| 32  | DF    | 201 | VAL  |
| 33  | DG    | 4   | ASP  |
| 33  | DG    | 5   | VAL  |
| 33  | DG    | 14  | GLU  |
| 33  | DG    | 16  | ARG  |
| 33  | DG    | 21  | ARG  |
| 33  | DG    | 22  | ARG  |
| 33  | DG    | 29  | TRP  |
| 33  | DG    | 35  | GLU  |
| 33  | DG    | 80  | PHE  |
| 33  | DG    | 83  | ARG  |
| 33  | DG    | 87  | PRO  |
| 33  | DG    | 92  | VAL  |
| 33  | DG    | 98  | ARG  |
| 33  | DG    | 101 | ILE  |
| 33  | DG    | 112 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | DG    | 113 | ARG  |
| 33  | DG    | 114 | ILE  |
| 33  | DG    | 116 | ASP  |
| 33  | DG    | 117 | PHE  |
| 33  | DG    | 125 | PHE  |
| 33  | DG    | 130 | ASN  |
| 33  | DG    | 131 | TYR  |
| 33  | DG    | 132 | ASN  |
| 33  | DG    | 139 | LEU  |
| 33  | DG    | 143 | GLU  |
| 33  | DG    | 147 | ASP  |
| 33  | DG    | 153 | ARG  |
| 33  | DG    | 157 | ILE  |
| 33  | DG    | 162 | THR  |
| 33  | DG    | 166 | ASP  |
| 34  | DH    | 13  | LYS  |
| 34  | DH    | 24  | VAL  |
| 34  | DH    | 25  | LYS  |
| 34  | DH    | 41  | MET  |
| 34  | DH    | 46  | GLU  |
| 34  | DH    | 50  | VAL  |
| 34  | DH    | 54  | ARG  |
| 34  | DH    | 70  | THR  |
| 34  | DH    | 72  | ILE  |
| 34  | DH    | 74  | ASN  |
| 34  | DH    | 86  | GLU  |
| 34  | DH    | 88  | LEU  |
| 34  | DH    | 95  | ARG  |
| 34  | DH    | 103 | LEU  |
| 34  | DH    | 106 | THR  |
| 34  | DH    | 111 | HIS  |
| 34  | DH    | 147 | ASN  |
| 34  | DH    | 152 | ARG  |
| 34  | DH    | 153 | LYS  |
| 34  | DH    | 157 | TYR  |
| 34  | DH    | 170 | ARG  |
| 35  | DI    | 2   | LYS  |
| 35  | DI    | 5   | LEU  |
| 35  | DI    | 6   | LEU  |
| 35  | DI    | 12  | LEU  |
| 35  | DI    | 43  | ASN  |
| 35  | DI    | 47  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | DI    | 51  | ILE  |
| 35  | DI    | 68  | LEU  |
| 35  | DI    | 72  | LEU  |
| 35  | DI    | 77  | LEU  |
| 35  | DI    | 86  | THR  |
| 35  | DI    | 102 | SER  |
| 35  | DI    | 109 | ILE  |
| 35  | DI    | 114 | LEU  |
| 35  | DI    | 122 | GLU  |
| 35  | DI    | 133 | HIS  |
| 35  | DI    | 138 | ILE  |
| 35  | DI    | 143 | SER  |
| 36  | DN    | 4   | TYR  |
| 36  | DN    | 23  | LEU  |
| 36  | DN    | 25  | ARG  |
| 36  | DN    | 28  | THR  |
| 36  | DN    | 34  | LEU  |
| 36  | DN    | 39  | ARG  |
| 36  | DN    | 41  | ASP  |
| 36  | DN    | 48  | MET  |
| 36  | DN    | 50  | ASP  |
| 36  | DN    | 54  | VAL  |
| 36  | DN    | 55  | VAL  |
| 36  | DN    | 56  | ASN  |
| 36  | DN    | 61  | ARG  |
| 36  | DN    | 63  | THR  |
| 36  | DN    | 73  | THR  |
| 36  | DN    | 88  | GLU  |
| 36  | DN    | 89  | LYS  |
| 36  | DN    | 98  | VAL  |
| 36  | DN    | 99  | LEU  |
| 36  | DN    | 119 | ARG  |
| 36  | DN    | 121 | LYS  |
| 36  | DN    | 127 | ASP  |
| 36  | DN    | 130 | HIS  |
| 36  | DN    | 134 | ARG  |
| 36  | DN    | 136 | GLU  |
| 37  | DO    | 1   | MET  |
| 37  | DO    | 7   | TYR  |
| 37  | DO    | 8   | LEU  |
| 37  | DO    | 9   | GLU  |
| 37  | DO    | 10  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DO    | 18  | LYS  |
| 37  | DO    | 19  | ILE  |
| 37  | DO    | 22  | ILE  |
| 37  | DO    | 35  | VAL  |
| 37  | DO    | 38  | VAL  |
| 37  | DO    | 42  | SER  |
| 37  | DO    | 45  | GLU  |
| 37  | DO    | 48  | PRO  |
| 37  | DO    | 49  | ARG  |
| 37  | DO    | 58  | VAL  |
| 37  | DO    | 59  | LYS  |
| 37  | DO    | 69  | ILE  |
| 37  | DO    | 75  | SER  |
| 37  | DO    | 79  | PHE  |
| 37  | DO    | 81  | ASP  |
| 37  | DO    | 87  | ILE  |
| 37  | DO    | 97  | ARG  |
| 37  | DO    | 98  | VAL  |
| 37  | DO    | 102 | VAL  |
| 37  | DO    | 117 | LEU  |
| 38  | DP    | 5   | ASP  |
| 38  | DP    | 6   | LEU  |
| 38  | DP    | 9   | ASN  |
| 38  | DP    | 13  | ASN  |
| 38  | DP    | 16  | ARG  |
| 38  | DP    | 18  | ARG  |
| 38  | DP    | 19  | VAL  |
| 38  | DP    | 21  | ARG  |
| 38  | DP    | 27  | HIS  |
| 38  | DP    | 30  | THR  |
| 38  | DP    | 39  | LYS  |
| 38  | DP    | 41  | ARG  |
| 38  | DP    | 47  | ASP  |
| 38  | DP    | 50  | ARG  |
| 38  | DP    | 51  | PHE  |
| 38  | DP    | 58  | THR  |
| 38  | DP    | 59  | LEU  |
| 38  | DP    | 61  | ARG  |
| 38  | DP    | 64  | LYS  |
| 38  | DP    | 68  | GLN  |
| 38  | DP    | 71  | VAL  |
| 38  | DP    | 83  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | DP    | 85  | LEU  |
| 38  | DP    | 87  | ASP  |
| 38  | DP    | 91  | PHE  |
| 38  | DP    | 95  | VAL  |
| 38  | DP    | 98  | GLU  |
| 38  | DP    | 105 | LEU  |
| 38  | DP    | 108 | LYS  |
| 38  | DP    | 112 | LEU  |
| 38  | DP    | 122 | PRO  |
| 38  | DP    | 125 | VAL  |
| 38  | DP    | 130 | PHE  |
| 39  | DQ    | 17  | LEU  |
| 39  | DQ    | 27  | VAL  |
| 39  | DQ    | 29  | PHE  |
| 39  | DQ    | 45  | GLN  |
| 39  | DQ    | 51  | ARG  |
| 39  | DQ    | 52  | VAL  |
| 39  | DQ    | 59  | ARG  |
| 39  | DQ    | 63  | LYS  |
| 39  | DQ    | 66  | ILE  |
| 39  | DQ    | 76  | LYS  |
| 39  | DQ    | 79  | LEU  |
| 39  | DQ    | 81  | VAL  |
| 39  | DQ    | 82  | ARG  |
| 39  | DQ    | 89  | ASN  |
| 39  | DQ    | 106 | VAL  |
| 39  | DQ    | 112 | GLU  |
| 39  | DQ    | 129 | THR  |
| 39  | DQ    | 134 | ARG  |
| 39  | DQ    | 135 | ASP  |
| 40  | DR    | 2   | ARG  |
| 40  | DR    | 4   | LEU  |
| 40  | DR    | 5   | LYS  |
| 40  | DR    | 8   | ARG  |
| 40  | DR    | 15  | SER  |
| 40  | DR    | 17  | ARG  |
| 40  | DR    | 27  | SER  |
| 40  | DR    | 28  | LEU  |
| 40  | DR    | 29  | LEU  |
| 40  | DR    | 30  | THR  |
| 40  | DR    | 33  | ARG  |
| 40  | DR    | 51  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | DR    | 54  | LEU  |
| 40  | DR    | 56  | LYS  |
| 40  | DR    | 57  | ARG  |
| 40  | DR    | 60  | LEU  |
| 40  | DR    | 67  | LEU  |
| 40  | DR    | 69  | ASP  |
| 40  | DR    | 71  | GLN  |
| 40  | DR    | 75  | LEU  |
| 40  | DR    | 79  | LEU  |
| 40  | DR    | 80  | PHE  |
| 40  | DR    | 81  | ASP  |
| 40  | DR    | 85  | PRO  |
| 40  | DR    | 88  | ARG  |
| 40  | DR    | 91  | GLN  |
| 40  | DR    | 94  | TYR  |
| 40  | DR    | 95  | THR  |
| 40  | DR    | 100 | LEU  |
| 40  | DR    | 103 | ARG  |
| 40  | DR    | 104 | ARG  |
| 40  | DR    | 111 | LEU  |
| 40  | DR    | 118 | GLU  |
| 41  | DS    | 12  | PHE  |
| 41  | DS    | 36  | TYR  |
| 41  | DS    | 58  | LEU  |
| 41  | DS    | 63  | THR  |
| 41  | DS    | 67  | ARG  |
| 41  | DS    | 73  | LEU  |
| 41  | DS    | 85  | VAL  |
| 41  | DS    | 87  | PHE  |
| 41  | DS    | 89  | ARG  |
| 41  | DS    | 92  | TYR  |
| 41  | DS    | 93  | LYS  |
| 41  | DS    | 97  | ARG  |
| 41  | DS    | 101 | LEU  |
| 41  | DS    | 106 | ARG  |
| 42  | DT    | 9   | LEU  |
| 42  | DT    | 11  | GLU  |
| 42  | DT    | 13  | ARG  |
| 42  | DT    | 14  | TYR  |
| 42  | DT    | 19  | LEU  |
| 42  | DT    | 22  | PHE  |
| 42  | DT    | 24  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DT    | 29  | ARG  |
| 42  | DT    | 30  | VAL  |
| 42  | DT    | 38  | ASN  |
| 42  | DT    | 41  | ARG  |
| 42  | DT    | 42  | ILE  |
| 42  | DT    | 46  | GLU  |
| 42  | DT    | 51  | ARG  |
| 42  | DT    | 55  | ASN  |
| 42  | DT    | 78  | LEU  |
| 42  | DT    | 80  | SER  |
| 42  | DT    | 81  | PRO  |
| 42  | DT    | 82  | LEU  |
| 42  | DT    | 84  | GLN  |
| 42  | DT    | 85  | LYS  |
| 42  | DT    | 86  | ILE  |
| 42  | DT    | 95  | ARG  |
| 42  | DT    | 96  | ARG  |
| 42  | DT    | 99  | LEU  |
| 42  | DT    | 100 | TYR  |
| 42  | DT    | 110 | ILE  |
| 42  | DT    | 113 | LYS  |
| 42  | DT    | 115 | ARG  |
| 42  | DT    | 119 | LYS  |
| 42  | DT    | 128 | GLU  |
| 42  | DT    | 132 | LYS  |
| 43  | DU    | 5   | LYS  |
| 43  | DU    | 15  | LYS  |
| 43  | DU    | 29  | SER  |
| 43  | DU    | 34  | LYS  |
| 43  | DU    | 52  | ARG  |
| 43  | DU    | 60  | LEU  |
| 43  | DU    | 63  | VAL  |
| 43  | DU    | 84  | LYS  |
| 43  | DU    | 92  | ARG  |
| 43  | DU    | 104 | GLN  |
| 43  | DU    | 105 | VAL  |
| 44  | DV    | 5   | VAL  |
| 44  | DV    | 18  | LEU  |
| 44  | DV    | 19  | LYS  |
| 44  | DV    | 21  | ARG  |
| 44  | DV    | 29  | PRO  |
| 44  | DV    | 32  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | DV    | 33  | VAL  |
| 44  | DV    | 38  | LEU  |
| 44  | DV    | 39  | LEU  |
| 44  | DV    | 40  | LEU  |
| 44  | DV    | 46  | VAL  |
| 44  | DV    | 49  | THR  |
| 44  | DV    | 56  | SER  |
| 44  | DV    | 61  | VAL  |
| 44  | DV    | 62  | LEU  |
| 44  | DV    | 68  | LYS  |
| 44  | DV    | 69  | LYS  |
| 44  | DV    | 71  | LEU  |
| 44  | DV    | 78  | LYS  |
| 44  | DV    | 89  | GLN  |
| 44  | DV    | 92  | THR  |
| 44  | DV    | 99  | ILE  |
| 45  | DW    | 6   | ILE  |
| 45  | DW    | 8   | ARG  |
| 45  | DW    | 11  | ARG  |
| 45  | DW    | 13  | SER  |
| 45  | DW    | 19  | LEU  |
| 45  | DW    | 23  | LEU  |
| 45  | DW    | 27  | LYS  |
| 45  | DW    | 50  | VAL  |
| 45  | DW    | 52  | GLU  |
| 45  | DW    | 57  | ASN  |
| 45  | DW    | 60  | ASN  |
| 45  | DW    | 63  | ASP  |
| 45  | DW    | 67  | ASP  |
| 45  | DW    | 70  | TYR  |
| 45  | DW    | 85  | VAL  |
| 45  | DW    | 86  | LEU  |
| 45  | DW    | 90  | ARG  |
| 45  | DW    | 96  | ILE  |
| 45  | DW    | 107 | LEU  |
| 46  | DX    | 5   | TYR  |
| 46  | DX    | 7   | VAL  |
| 46  | DX    | 8   | ILE  |
| 46  | DX    | 15  | GLU  |
| 46  | DX    | 27  | THR  |
| 46  | DX    | 51  | VAL  |
| 46  | DX    | 52  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | DX    | 53  | LYS  |
| 46  | DX    | 57  | LEU  |
| 46  | DX    | 60  | ARG  |
| 46  | DX    | 68  | ARG  |
| 46  | DX    | 70  | LEU  |
| 46  | DX    | 76  | ARG  |
| 46  | DX    | 78  | LYS  |
| 46  | DX    | 80  | ILE  |
| 46  | DX    | 83  | VAL  |
| 47  | DY    | 6   | HIS  |
| 47  | DY    | 7   | VAL  |
| 47  | DY    | 8   | LYS  |
| 47  | DY    | 19  | LYS  |
| 47  | DY    | 28  | LYS  |
| 47  | DY    | 29  | GLU  |
| 47  | DY    | 32  | PRO  |
| 47  | DY    | 42  | VAL  |
| 47  | DY    | 47  | LYS  |
| 47  | DY    | 53  | PRO  |
| 47  | DY    | 55  | TYR  |
| 47  | DY    | 56  | PRO  |
| 47  | DY    | 60  | PHE  |
| 47  | DY    | 67  | LEU  |
| 47  | DY    | 71  | LYS  |
| 47  | DY    | 72  | VAL  |
| 47  | DY    | 76  | CYS  |
| 47  | DY    | 77  | PRO  |
| 47  | DY    | 79  | CYS  |
| 47  | DY    | 89  | PHE  |
| 47  | DY    | 90  | LEU  |
| 48  | DZ    | 7   | TYR  |
| 48  | DZ    | 18  | ARG  |
| 48  | DZ    | 22  | LYS  |
| 48  | DZ    | 31  | HIS  |
| 48  | DZ    | 40  | LEU  |
| 48  | DZ    | 52  | ILE  |
| 48  | DZ    | 60  | LEU  |
| 48  | DZ    | 72  | GLN  |
| 48  | DZ    | 78  | ARG  |
| 48  | DZ    | 79  | ARG  |
| 48  | DZ    | 90  | LEU  |
| 48  | DZ    | 92  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | DZ    | 103 | PHE  |
| 48  | DZ    | 118 | GLU  |
| 48  | DZ    | 128 | SER  |
| 48  | DZ    | 130 | ARG  |
| 48  | DZ    | 131 | ASN  |
| 48  | DZ    | 144 | GLU  |
| 48  | DZ    | 147 | ASP  |
| 48  | DZ    | 149 | LEU  |
| 49  | D0    | 5   | LYS  |
| 49  | D0    | 20  | ARG  |
| 49  | D0    | 30  | VAL  |
| 49  | D0    | 41  | ARG  |
| 49  | D0    | 64  | ASP  |
| 49  | D0    | 70  | GLN  |
| 49  | D0    | 75  | LEU  |
| 49  | D0    | 84  | LEU  |
| 50  | D1    | 21  | ARG  |
| 50  | D1    | 30  | VAL  |
| 50  | D1    | 38  | SER  |
| 50  | D1    | 40  | ARG  |
| 50  | D1    | 45  | ASN  |
| 50  | D1    | 46  | LEU  |
| 50  | D1    | 47  | GLN  |
| 50  | D1    | 50  | ARG  |
| 50  | D1    | 58  | ILE  |
| 50  | D1    | 59  | THR  |
| 50  | D1    | 61  | ARG  |
| 50  | D1    | 80  | LEU  |
| 50  | D1    | 82  | LEU  |
| 50  | D1    | 90  | ILE  |
| 50  | D1    | 95  | LEU  |
| 51  | D2    | 2   | LYS  |
| 51  | D2    | 3   | LEU  |
| 51  | D2    | 4   | SER  |
| 51  | D2    | 5   | GLU  |
| 51  | D2    | 17  | SER  |
| 51  | D2    | 20  | GLU  |
| 51  | D2    | 32  | LEU  |
| 51  | D2    | 44  | LEU  |
| 51  | D2    | 53  | LEU  |
| 51  | D2    | 57  | ILE  |
| 51  | D2    | 60  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | D2    | 63  | VAL  |
| 51  | D2    | 69  | ARG  |
| 52  | D3    | 4   | LEU  |
| 52  | D3    | 6   | VAL  |
| 52  | D3    | 8   | LEU  |
| 52  | D3    | 18  | ASP  |
| 52  | D3    | 23  | LEU  |
| 52  | D3    | 38  | GLU  |
| 52  | D3    | 52  | HIS  |
| 53  | D4    | 36  | VAL  |
| 53  | D4    | 56  | GLU  |
| 54  | D5    | 11  | THR  |
| 54  | D5    | 23  | HIS  |
| 54  | D5    | 25  | LEU  |
| 54  | D5    | 33  | CYS  |
| 54  | D5    | 36  | CYS  |
| 54  | D5    | 37  | LYS  |
| 54  | D5    | 40  | LYS  |
| 54  | D5    | 49  | CYS  |
| 54  | D5    | 56  | LYS  |
| 55  | D6    | 8   | LYS  |
| 55  | D6    | 10  | LEU  |
| 55  | D6    | 11  | LEU  |
| 55  | D6    | 13  | CYS  |
| 55  | D6    | 18  | ARG  |
| 55  | D6    | 19  | ARG  |
| 55  | D6    | 31  | PRO  |
| 55  | D6    | 32  | ASN  |
| 55  | D6    | 33  | LYS  |
| 55  | D6    | 36  | LEU  |
| 55  | D6    | 37  | ARG  |
| 55  | D6    | 40  | CYS  |
| 55  | D6    | 41  | PRO  |
| 55  | D6    | 42  | TRP  |
| 55  | D6    | 43  | CYS  |
| 55  | D6    | 47  | THR  |
| 56  | D7    | 1   | MET  |
| 56  | D7    | 4   | THR  |
| 56  | D7    | 8   | ASN  |
| 56  | D7    | 41  | ARG  |
| 56  | D7    | 42  | LEU  |
| 57  | D8    | 8   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | D8    | 16  | ILE  |
| 57  | D8    | 19  | SER  |
| 57  | D8    | 30  | ARG  |
| 57  | D8    | 32  | LEU  |
| 57  | D8    | 33  | ASN  |
| 57  | D8    | 34  | TRP  |
| 57  | D8    | 42  | ARG  |
| 57  | D8    | 44  | LYS  |
| 57  | D8    | 52  | LYS  |
| 57  | D8    | 54  | GLU  |
| 57  | D8    | 56  | GLU  |
| 57  | D8    | 61  | LEU  |
| 57  | D8    | 63  | PRO  |
| 58  | D9    | 2   | LYS  |
| 58  | D9    | 9   | ARG  |
| 58  | D9    | 18  | ARG  |
| 58  | D9    | 28  | GLU  |
| 58  | D9    | 29  | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (293) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 45  | GLN  |
| 2   | AB    | 78  | GLN  |
| 2   | AB    | 104 | ASN  |
| 2   | AB    | 110 | GLN  |
| 2   | AB    | 204 | ASN  |
| 2   | AB    | 224 | GLN  |
| 3   | AC    | 6   | HIS  |
| 3   | AC    | 28  | GLN  |
| 3   | AC    | 170 | GLN  |
| 4   | AD    | 119 | GLN  |
| 4   | AD    | 123 | HIS  |
| 4   | AD    | 125 | HIS  |
| 4   | AD    | 201 | GLN  |
| 5   | AE    | 72  | GLN  |
| 5   | AE    | 73  | ASN  |
| 5   | AE    | 78  | HIS  |
| 6   | AF    | 16  | GLN  |
| 6   | AF    | 18  | GLN  |
| 6   | AF    | 27  | GLN  |
| 6   | AF    | 32  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AF    | 64  | GLN  |
| 6   | AF    | 73  | ASN  |
| 6   | AF    | 94  | GLN  |
| 6   | AF    | 100 | ASN  |
| 7   | AG    | 13  | GLN  |
| 7   | AG    | 96  | GLN  |
| 7   | AG    | 97  | GLN  |
| 7   | AG    | 148 | ASN  |
| 9   | AI    | 23  | ASN  |
| 9   | AI    | 31  | GLN  |
| 9   | AI    | 73  | GLN  |
| 9   | AI    | 89  | ASN  |
| 9   | AI    | 124 | GLN  |
| 10  | AJ    | 56  | HIS  |
| 10  | AJ    | 62  | HIS  |
| 11  | AK    | 22  | HIS  |
| 11  | AK    | 38  | ASN  |
| 11  | AK    | 99  | GLN  |
| 11  | AK    | 117 | ASN  |
| 12  | AL    | 5   | ASN  |
| 12  | AL    | 6   | GLN  |
| 12  | AL    | 46  | ASN  |
| 12  | AL    | 73  | ASN  |
| 12  | AL    | 96  | HIS  |
| 13  | AM    | 40  | ASN  |
| 13  | AM    | 77  | ASN  |
| 13  | AM    | 101 | GLN  |
| 15  | AO    | 37  | ASN  |
| 15  | AO    | 62  | GLN  |
| 16  | AP    | 76  | GLN  |
| 16  | AP    | 82  | GLN  |
| 17  | AQ    | 16  | GLN  |
| 17  | AQ    | 26  | GLN  |
| 17  | AQ    | 93  | GLN  |
| 20  | AT    | 18  | GLN  |
| 20  | AT    | 26  | ASN  |
| 20  | AT    | 75  | ASN  |
| 30  | BD    | 58  | HIS  |
| 30  | BD    | 96  | HIS  |
| 30  | BD    | 115 | GLN  |
| 30  | BD    | 166 | GLN  |
| 30  | BD    | 186 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BD    | 198 | ASN  |
| 30  | BD    | 220 | HIS  |
| 30  | BD    | 227 | ASN  |
| 30  | BD    | 253 | GLN  |
| 31  | BE    | 35  | GLN  |
| 31  | BE    | 54  | GLN  |
| 31  | BE    | 55  | ASN  |
| 31  | BE    | 66  | HIS  |
| 31  | BE    | 121 | ASN  |
| 31  | BE    | 132 | HIS  |
| 32  | BF    | 69  | HIS  |
| 32  | BF    | 75  | HIS  |
| 32  | BF    | 160 | ASN  |
| 32  | BF    | 169 | ASN  |
| 32  | BF    | 203 | GLN  |
| 32  | BF    | 204 | ASN  |
| 33  | BG    | 26  | GLN  |
| 33  | BG    | 66  | GLN  |
| 33  | BG    | 108 | ASN  |
| 34  | BH    | 65  | HIS  |
| 34  | BH    | 147 | ASN  |
| 34  | BH    | 158 | HIS  |
| 35  | BI    | 17  | GLN  |
| 35  | BI    | 28  | ASN  |
| 35  | BI    | 43  | ASN  |
| 35  | BI    | 54  | GLN  |
| 35  | BI    | 105 | HIS  |
| 35  | BI    | 133 | HIS  |
| 36  | BN    | 56  | ASN  |
| 36  | BN    | 69  | GLN  |
| 36  | BN    | 94  | HIS  |
| 36  | BN    | 130 | HIS  |
| 36  | BN    | 131 | GLN  |
| 37  | BO    | 3   | GLN  |
| 37  | BO    | 13  | ASN  |
| 37  | BO    | 82  | ASN  |
| 38  | BP    | 9   | ASN  |
| 38  | BP    | 27  | HIS  |
| 38  | BP    | 38  | GLN  |
| 38  | BP    | 68  | GLN  |
| 38  | BP    | 84  | ASN  |
| 38  | BP    | 128 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BQ    | 12  | GLN  |
| 39  | BQ    | 46  | GLN  |
| 39  | BQ    | 57  | HIS  |
| 39  | BQ    | 123 | HIS  |
| 40  | BR    | 3   | HIS  |
| 40  | BR    | 16  | HIS  |
| 40  | BR    | 23  | ASN  |
| 40  | BR    | 24  | GLN  |
| 40  | BR    | 50  | HIS  |
| 40  | BR    | 53  | HIS  |
| 40  | BR    | 71  | GLN  |
| 41  | BS    | 68  | GLN  |
| 42  | BT    | 90  | GLN  |
| 43  | BU    | 49  | HIS  |
| 43  | BU    | 72  | HIS  |
| 43  | BU    | 104 | GLN  |
| 43  | BU    | 117 | GLN  |
| 44  | BV    | 11  | GLN  |
| 45  | BW    | 34  | ASN  |
| 45  | BW    | 40  | ASN  |
| 45  | BW    | 57  | ASN  |
| 45  | BW    | 61  | ASN  |
| 45  | BW    | 62  | HIS  |
| 45  | BW    | 102 | HIS  |
| 45  | BW    | 111 | HIS  |
| 46  | BX    | 31  | HIS  |
| 46  | BX    | 41  | ASN  |
| 46  | BX    | 55  | ASN  |
| 48  | BZ    | 33  | ASN  |
| 48  | BZ    | 54  | HIS  |
| 48  | BZ    | 117 | GLN  |
| 48  | BZ    | 131 | ASN  |
| 49  | B0    | 29  | GLN  |
| 50  | B1    | 19  | GLN  |
| 50  | B1    | 45  | ASN  |
| 51  | B2    | 9   | GLN  |
| 51  | B2    | 43  | GLN  |
| 51  | B2    | 46  | GLN  |
| 52  | B3    | 19  | GLN  |
| 52  | B3    | 33  | GLN  |
| 52  | B3    | 46  | ASN  |
| 53  | B4    | 46  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | B5    | 4   | HIS  |
| 54  | B5    | 43  | HIS  |
| 55  | B6    | 20  | ASN  |
| 55  | B6    | 26  | ASN  |
| 56  | B7    | 6   | GLN  |
| 56  | B7    | 8   | ASN  |
| 57  | B8    | 31  | HIS  |
| 57  | B8    | 33  | ASN  |
| 57  | B8    | 35  | GLN  |
| 57  | B8    | 43  | GLN  |
| 58  | B9    | 29  | ASN  |
| 58  | B9    | 34  | GLN  |
| 2   | CB    | 16  | HIS  |
| 2   | CB    | 40  | HIS  |
| 2   | CB    | 110 | GLN  |
| 2   | CB    | 135 | GLN  |
| 2   | CB    | 146 | GLN  |
| 3   | CC    | 6   | HIS  |
| 3   | CC    | 28  | GLN  |
| 3   | CC    | 69  | HIS  |
| 3   | CC    | 123 | GLN  |
| 3   | CC    | 170 | GLN  |
| 4   | CD    | 62  | GLN  |
| 4   | CD    | 160 | GLN  |
| 4   | CD    | 161 | ASN  |
| 5   | CE    | 73  | ASN  |
| 6   | CF    | 7   | ASN  |
| 6   | CF    | 18  | GLN  |
| 6   | CF    | 27  | GLN  |
| 6   | CF    | 32  | ASN  |
| 6   | CF    | 94  | GLN  |
| 6   | CF    | 100 | ASN  |
| 7   | CG    | 11  | GLN  |
| 7   | CG    | 28  | ASN  |
| 7   | CG    | 84  | ASN  |
| 7   | CG    | 96  | GLN  |
| 7   | CG    | 97  | GLN  |
| 8   | CH    | 15  | ASN  |
| 9   | CI    | 23  | ASN  |
| 9   | CI    | 73  | GLN  |
| 10  | CJ    | 13  | HIS  |
| 10  | CJ    | 78  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | CK    | 13  | GLN  |
| 11  | CK    | 38  | ASN  |
| 12  | CL    | 5   | ASN  |
| 12  | CL    | 72  | HIS  |
| 13  | CM    | 77  | ASN  |
| 13  | CM    | 92  | HIS  |
| 13  | CM    | 101 | GLN  |
| 13  | CM    | 106 | ASN  |
| 15  | CO    | 9   | GLN  |
| 15  | CO    | 13  | GLN  |
| 15  | CO    | 37  | ASN  |
| 15  | CO    | 50  | HIS  |
| 15  | CO    | 71  | GLN  |
| 16  | CP    | 82  | GLN  |
| 17  | CQ    | 93  | GLN  |
| 18  | CR    | 36  | ASN  |
| 19  | CS    | 14  | HIS  |
| 19  | CS    | 23  | ASN  |
| 19  | CS    | 47  | HIS  |
| 19  | CS    | 53  | ASN  |
| 19  | CS    | 57  | HIS  |
| 20  | CT    | 26  | ASN  |
| 30  | DD    | 87  | ASN  |
| 30  | DD    | 115 | GLN  |
| 30  | DD    | 186 | HIS  |
| 30  | DD    | 220 | HIS  |
| 30  | DD    | 253 | GLN  |
| 31  | DE    | 54  | GLN  |
| 31  | DE    | 55  | ASN  |
| 31  | DE    | 66  | HIS  |
| 31  | DE    | 129 | HIS  |
| 31  | DE    | 192 | ASN  |
| 32  | DF    | 8   | GLN  |
| 32  | DF    | 31  | HIS  |
| 32  | DF    | 75  | HIS  |
| 33  | DG    | 41  | GLN  |
| 33  | DG    | 132 | ASN  |
| 34  | DH    | 61  | HIS  |
| 34  | DH    | 74  | ASN  |
| 34  | DH    | 143 | GLN  |
| 34  | DH    | 147 | ASN  |
| 35  | DI    | 17  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | DI    | 105 | HIS  |
| 36  | DN    | 38  | HIS  |
| 36  | DN    | 56  | ASN  |
| 36  | DN    | 69  | GLN  |
| 36  | DN    | 131 | GLN  |
| 37  | DO    | 5   | GLN  |
| 37  | DO    | 82  | ASN  |
| 38  | DP    | 9   | ASN  |
| 38  | DP    | 13  | ASN  |
| 38  | DP    | 27  | HIS  |
| 38  | DP    | 35  | HIS  |
| 38  | DP    | 38  | GLN  |
| 38  | DP    | 68  | GLN  |
| 38  | DP    | 84  | ASN  |
| 38  | DP    | 128 | HIS  |
| 39  | DQ    | 12  | GLN  |
| 39  | DQ    | 45  | GLN  |
| 40  | DR    | 16  | HIS  |
| 40  | DR    | 23  | ASN  |
| 40  | DR    | 24  | GLN  |
| 40  | DR    | 31  | HIS  |
| 40  | DR    | 53  | HIS  |
| 40  | DR    | 71  | GLN  |
| 41  | DS    | 16  | ASN  |
| 41  | DS    | 34  | HIS  |
| 41  | DS    | 68  | GLN  |
| 42  | DT    | 43  | GLN  |
| 42  | DT    | 90  | GLN  |
| 42  | DT    | 123 | GLN  |
| 43  | DU    | 49  | HIS  |
| 43  | DU    | 81  | HIS  |
| 44  | DV    | 11  | GLN  |
| 44  | DV    | 80  | GLN  |
| 45  | DW    | 34  | ASN  |
| 45  | DW    | 57  | ASN  |
| 45  | DW    | 102 | HIS  |
| 46  | DX    | 41  | ASN  |
| 46  | DX    | 58  | HIS  |
| 47  | DY    | 43  | ASN  |
| 48  | DZ    | 53  | HIS  |
| 48  | DZ    | 72  | GLN  |
| 48  | DZ    | 74  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | DZ    | 117 | GLN  |
| 48  | DZ    | 120 | HIS  |
| 48  | DZ    | 131 | ASN  |
| 49  | D0    | 29  | GLN  |
| 49  | D0    | 70  | GLN  |
| 50  | D1    | 45  | ASN  |
| 51  | D2    | 43  | GLN  |
| 51  | D2    | 47  | ASN  |
| 52  | D3    | 19  | GLN  |
| 52  | D3    | 32  | GLN  |
| 52  | D3    | 46  | ASN  |
| 52  | D3    | 52  | HIS  |
| 53  | D4    | 46  | ASN  |
| 54  | D5    | 4   | HIS  |
| 54  | D5    | 43  | HIS  |
| 55  | D6    | 32  | ASN  |
| 56  | D7    | 8   | ASN  |
| 56  | D7    | 36  | GLN  |
| 57  | D8    | 31  | HIS  |
| 57  | D8    | 33  | ASN  |
| 58  | D9    | 29  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1493/1509 (98%) | 351 (23%)         | 0               |
| 1   | CA    | 1493/1509 (98%) | 365 (24%)         | 0               |
| 22  | AV    | 9/30 (30%)      | 0                 | 0               |
| 22  | CV    | 9/30 (30%)      | 0                 | 0               |
| 23  | AW    | 74/75 (98%)     | 17 (22%)          | 0               |
| 23  | CW    | 74/75 (98%)     | 16 (21%)          | 0               |
| 24  | AX    | 76/77 (98%)     | 19 (25%)          | 0               |
| 24  | CX    | 76/77 (98%)     | 19 (25%)          | 0               |
| 25  | AY    | 74/75 (98%)     | 23 (31%)          | 0               |
| 25  | CY    | 74/75 (98%)     | 22 (29%)          | 0               |
| 27  | BA    | 2792/2915 (95%) | 798 (28%)         | 0               |
| 27  | DA    | 2792/2915 (95%) | 905 (32%)         | 0               |
| 28  | BB    | 116/122 (95%)   | 26 (22%)          | 0               |
| 28  | DB    | 116/122 (95%)   | 28 (24%)          | 0               |
| All | All   | 9268/9606 (96%) | 2589 (27%)        | 0               |

All (2589) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | AA    | 8      | A    |
| 1   | AA    | 9      | G    |
| 1   | AA    | 13     | U    |
| 1   | AA    | 31     | G    |
| 1   | AA    | 32     | A    |
| 1   | AA    | 39     | G    |
| 1   | AA    | 41     | G    |
| 1   | AA    | 47     | C    |
| 1   | AA    | 48     | C    |
| 1   | AA    | 51     | A    |
| 1   | AA    | 52     | G    |
| 1   | AA    | 53     | A    |
| 1   | AA    | 61     | G    |
| 1   | AA    | 64     | G    |
| 1   | AA    | 65     | U    |
| 1   | AA    | 107    | G    |
| 1   | AA    | 110    | C    |
| 1   | AA    | 114    | U    |
| 1   | AA    | 116    | A    |
| 1   | AA    | 120    | A    |
| 1   | AA    | 121    | C    |
| 1   | AA    | 129(A) | G    |
| 1   | AA    | 131    | C    |
| 1   | AA    | 132    | C    |
| 1   | AA    | 137    | C    |
| 1   | AA    | 143    | A    |
| 1   | AA    | 146    | G    |
| 1   | AA    | 170    | U    |
| 1   | AA    | 174    | C    |
| 1   | AA    | 181    | G    |
| 1   | AA    | 182    | U    |
| 1   | AA    | 183    | G    |
| 1   | AA    | 189(F) | U    |
| 1   | AA    | 189(H) | G    |
| 1   | AA    | 189(I) | G    |
| 1   | AA    | 195    | A    |
| 1   | AA    | 198    | G    |
| 1   | AA    | 199    | G    |
| 1   | AA    | 203    | U    |
| 1   | AA    | 204    | U    |
| 1   | AA    | 216    | G    |
| 1   | AA    | 220    | G    |
| 1   | AA    | 237    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 244 | U    |
| 1   | AA    | 247 | G    |
| 1   | AA    | 251 | G    |
| 1   | AA    | 253 | U    |
| 1   | AA    | 258 | G    |
| 1   | AA    | 262 | A    |
| 1   | AA    | 266 | G    |
| 1   | AA    | 267 | C    |
| 1   | AA    | 274 | A    |
| 1   | AA    | 275 | G    |
| 1   | AA    | 279 | A    |
| 1   | AA    | 280 | C    |
| 1   | AA    | 281 | G    |
| 1   | AA    | 287 | U    |
| 1   | AA    | 289 | G    |
| 1   | AA    | 306 | G    |
| 1   | AA    | 316 | G    |
| 1   | AA    | 328 | C    |
| 1   | AA    | 330 | C    |
| 1   | AA    | 332 | G    |
| 1   | AA    | 344 | A    |
| 1   | AA    | 345 | C    |
| 1   | AA    | 346 | G    |
| 1   | AA    | 347 | G    |
| 1   | AA    | 352 | C    |
| 1   | AA    | 353 | A    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 358 | U    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 369 | C    |
| 1   | AA    | 373 | A    |
| 1   | AA    | 374 | A    |
| 1   | AA    | 389 | A    |
| 1   | AA    | 390 | C    |
| 1   | AA    | 397 | A    |
| 1   | AA    | 406 | G    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 413 | G    |
| 1   | AA    | 414 | A    |
| 1   | AA    | 415 | A    |
| 1   | AA    | 421 | U    |
| 1   | AA    | 422 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 423 | G    |
| 1   | AA    | 424 | G    |
| 1   | AA    | 428 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 435 | C    |
| 1   | AA    | 439 | A    |
| 1   | AA    | 442 | C    |
| 1   | AA    | 451 | A    |
| 1   | AA    | 452 | A    |
| 1   | AA    | 453 | A    |
| 1   | AA    | 454 | C    |
| 1   | AA    | 455 | C    |
| 1   | AA    | 461 | A    |
| 1   | AA    | 470 | C    |
| 1   | AA    | 471 | G    |
| 1   | AA    | 472 | A    |
| 1   | AA    | 482 | A    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | G    |
| 1   | AA    | 486 | U    |
| 1   | AA    | 487 | A    |
| 1   | AA    | 495 | A    |
| 1   | AA    | 496 | A    |
| 1   | AA    | 498 | U    |
| 1   | AA    | 499 | A    |
| 1   | AA    | 508 | C    |
| 1   | AA    | 509 | A    |
| 1   | AA    | 511 | C    |
| 1   | AA    | 518 | C    |
| 1   | AA    | 521 | G    |
| 1   | AA    | 527 | G    |
| 1   | AA    | 531 | U    |
| 1   | AA    | 532 | A    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 534 | U    |
| 1   | AA    | 535 | A    |
| 1   | AA    | 548 | G    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 560 | U    |
| 1   | AA    | 562 | C    |
| 1   | AA    | 566 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 569 | C    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 575 | G    |
| 1   | AA    | 576 | G    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 578 | C    |
| 1   | AA    | 579 | G    |
| 1   | AA    | 595 | G    |
| 1   | AA    | 596 | C    |
| 1   | AA    | 607 | A    |
| 1   | AA    | 623 | C    |
| 1   | AA    | 632 | A    |
| 1   | AA    | 642 | A    |
| 1   | AA    | 653 | A    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 666 | G    |
| 1   | AA    | 687 | A    |
| 1   | AA    | 688 | G    |
| 1   | AA    | 693 | G    |
| 1   | AA    | 699 | C    |
| 1   | AA    | 701 | C    |
| 1   | AA    | 702 | A    |
| 1   | AA    | 703 | G    |
| 1   | AA    | 717 | C    |
| 1   | AA    | 718 | G    |
| 1   | AA    | 721 | G    |
| 1   | AA    | 722 | A    |
| 1   | AA    | 724 | G    |
| 1   | AA    | 731 | G    |
| 1   | AA    | 733 | A    |
| 1   | AA    | 748 | C    |
| 1   | AA    | 749 | C    |
| 1   | AA    | 752 | G    |
| 1   | AA    | 753 | A    |
| 1   | AA    | 755 | G    |
| 1   | AA    | 759 | A    |
| 1   | AA    | 767 | A    |
| 1   | AA    | 773 | G    |
| 1   | AA    | 777 | A    |
| 1   | AA    | 790 | A    |
| 1   | AA    | 793 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 801 | U    |
| 1   | AA    | 815 | A    |
| 1   | AA    | 816 | A    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 818 | G    |
| 1   | AA    | 819 | A    |
| 1   | AA    | 821 | G    |
| 1   | AA    | 828 | A    |
| 1   | AA    | 839 | U    |
| 1   | AA    | 841 | U    |
| 1   | AA    | 848 | C    |
| 1   | AA    | 853 | G    |
| 1   | AA    | 855 | G    |
| 1   | AA    | 859 | A    |
| 1   | AA    | 871 | U    |
| 1   | AA    | 884 | U    |
| 1   | AA    | 885 | G    |
| 1   | AA    | 890 | G    |
| 1   | AA    | 902 | G    |
| 1   | AA    | 914 | A    |
| 1   | AA    | 922 | G    |
| 1   | AA    | 926 | G    |
| 1   | AA    | 927 | G    |
| 1   | AA    | 934 | C    |
| 1   | AA    | 935 | A    |
| 1   | AA    | 954 | G    |
| 1   | AA    | 960 | U    |
| 1   | AA    | 961 | U    |
| 1   | AA    | 966 | G    |
| 1   | AA    | 968 | A    |
| 1   | AA    | 969 | A    |
| 1   | AA    | 972 | C    |
| 1   | AA    | 974 | A    |
| 1   | AA    | 975 | A    |
| 1   | AA    | 976 | G    |
| 1   | AA    | 977 | A    |
| 1   | AA    | 978 | A    |
| 1   | AA    | 980 | C    |
| 1   | AA    | 981 | U    |
| 1   | AA    | 982 | U    |
| 1   | AA    | 983 | A    |
| 1   | AA    | 984 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 991     | U    |
| 1   | AA    | 992     | U    |
| 1   | AA    | 993     | G    |
| 1   | AA    | 1001(A) | G    |
| 1   | AA    | 1005    | A    |
| 1   | AA    | 1006    | C    |
| 1   | AA    | 1009    | G    |
| 1   | AA    | 1016    | A    |
| 1   | AA    | 1017    | G    |
| 1   | AA    | 1027    | C    |
| 1   | AA    | 1030    | C    |
| 1   | AA    | 1030(A) | G    |
| 1   | AA    | 1030(B) | C    |
| 1   | AA    | 1030(C) | G    |
| 1   | AA    | 1045    | C    |
| 1   | AA    | 1050    | G    |
| 1   | AA    | 1053    | G    |
| 1   | AA    | 1054    | C    |
| 1   | AA    | 1062    | U    |
| 1   | AA    | 1064    | G    |
| 1   | AA    | 1065    | U    |
| 1   | AA    | 1066    | C    |
| 1   | AA    | 1068    | G    |
| 1   | AA    | 1070    | U    |
| 1   | AA    | 1085    | U    |
| 1   | AA    | 1086    | U    |
| 1   | AA    | 1087    | G    |
| 1   | AA    | 1094    | G    |
| 1   | AA    | 1095    | U    |
| 1   | AA    | 1101    | A    |
| 1   | AA    | 1102    | A    |
| 1   | AA    | 1117    | G    |
| 1   | AA    | 1118    | C    |
| 1   | AA    | 1125    | U    |
| 1   | AA    | 1126    | U    |
| 1   | AA    | 1127    | G    |
| 1   | AA    | 1129    | C    |
| 1   | AA    | 1130    | A    |
| 1   | AA    | 1136    | U    |
| 1   | AA    | 1137    | C    |
| 1   | AA    | 1139    | G    |
| 1   | AA    | 1140    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1141 | C    |
| 1   | AA    | 1142 | G    |
| 1   | AA    | 1146 | A    |
| 1   | AA    | 1147 | C    |
| 1   | AA    | 1148 | U    |
| 1   | AA    | 1153 | C    |
| 1   | AA    | 1154 | G    |
| 1   | AA    | 1158 | C    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1160 | G    |
| 1   | AA    | 1181 | G    |
| 1   | AA    | 1183 | A    |
| 1   | AA    | 1184 | G    |
| 1   | AA    | 1190 | G    |
| 1   | AA    | 1196 | U    |
| 1   | AA    | 1197 | G    |
| 1   | AA    | 1200 | C    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1202 | G    |
| 1   | AA    | 1212 | U    |
| 1   | AA    | 1213 | A    |
| 1   | AA    | 1214 | C    |
| 1   | AA    | 1225 | A    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1227 | A    |
| 1   | AA    | 1238 | A    |
| 1   | AA    | 1239 | A    |
| 1   | AA    | 1240 | U    |
| 1   | AA    | 1241 | G    |
| 1   | AA    | 1242 | C    |
| 1   | AA    | 1249 | C    |
| 1   | AA    | 1253 | G    |
| 1   | AA    | 1256 | A    |
| 1   | AA    | 1257 | U    |
| 1   | AA    | 1262 | C    |
| 1   | AA    | 1267 | C    |
| 1   | AA    | 1273 | G    |
| 1   | AA    | 1278 | U    |
| 1   | AA    | 1279 | A    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1281 | U    |
| 1   | AA    | 1285 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 1286    | A    |
| 1   | AA    | 1287    | A    |
| 1   | AA    | 1296    | C    |
| 1   | AA    | 1297    | C    |
| 1   | AA    | 1298    | C    |
| 1   | AA    | 1299    | A    |
| 1   | AA    | 1300    | G    |
| 1   | AA    | 1301    | U    |
| 1   | AA    | 1302    | U    |
| 1   | AA    | 1305    | G    |
| 1   | AA    | 1306    | A    |
| 1   | AA    | 1317    | C    |
| 1   | AA    | 1320    | C    |
| 1   | AA    | 1322    | C    |
| 1   | AA    | 1323    | G    |
| 1   | AA    | 1325    | C    |
| 1   | AA    | 1331    | G    |
| 1   | AA    | 1335    | C    |
| 1   | AA    | 1336    | C    |
| 1   | AA    | 1337    | G    |
| 1   | AA    | 1347    | G    |
| 1   | AA    | 1353    | G    |
| 1   | AA    | 1363(A) | A    |
| 1   | AA    | 1364    | U    |
| 1   | AA    | 1365    | G    |
| 1   | AA    | 1370    | G    |
| 1   | AA    | 1379    | G    |
| 1   | AA    | 1381    | U    |
| 1   | AA    | 1382    | C    |
| 1   | AA    | 1395    | C    |
| 1   | AA    | 1397    | C    |
| 1   | AA    | 1398    | A    |
| 1   | AA    | 1399    | C    |
| 1   | AA    | 1400    | C    |
| 1   | AA    | 1419    | G    |
| 1   | AA    | 1425    | U    |
| 1   | AA    | 1438    | G    |
| 1   | AA    | 1442    | G    |
| 1   | AA    | 1442(A) | G    |
| 1   | AA    | 1442(B) | A    |
| 1   | AA    | 1443    | G    |
| 1   | AA    | 1447    | A    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | AA    | 1452  | C    |
| 1   | AA    | 1456  | G    |
| 1   | AA    | 1487  | G    |
| 1   | AA    | 1492  | A    |
| 1   | AA    | 1498  | U    |
| 1   | AA    | 1499  | A    |
| 1   | AA    | 1504  | G    |
| 1   | AA    | 1506  | U    |
| 1   | AA    | 1507  | A    |
| 1   | AA    | 1517  | G    |
| 1   | AA    | 1519  | A    |
| 1   | AA    | 1520  | G    |
| 1   | AA    | 1529  | G    |
| 1   | AA    | 1531  | A    |
| 23  | AW    | 2     | G    |
| 23  | AW    | 5     | G    |
| 23  | AW    | 7     | A    |
| 23  | AW    | 8     | U    |
| 23  | AW    | 12    | C    |
| 23  | AW    | 16    | C    |
| 23  | AW    | 17    | G    |
| 23  | AW    | 18    | G    |
| 23  | AW    | 20    | A    |
| 23  | AW    | 23    | G    |
| 23  | AW    | 31    | U    |
| 23  | AW    | 43    | C    |
| 23  | AW    | 45    | U    |
| 23  | AW    | 48    | C    |
| 23  | AW    | 72    | G    |
| 23  | AW    | 73    | C    |
| 23  | AW    | 74    | C    |
| 24  | AX    | 3     | C    |
| 24  | AX    | 8     | U    |
| 24  | AX    | 13    | C    |
| 24  | AX    | 17    | C    |
| 24  | AX    | 17(B) | U    |
| 24  | AX    | 18    | G    |
| 24  | AX    | 19    | G    |
| 24  | AX    | 20    | U    |
| 24  | AX    | 21    | A    |
| 24  | AX    | 47    | U    |
| 24  | AX    | 48    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | AX    | 49  | G    |
| 24  | AX    | 59  | A    |
| 24  | AX    | 60  | U    |
| 24  | AX    | 63  | G    |
| 24  | AX    | 65  | C    |
| 24  | AX    | 73  | A    |
| 24  | AX    | 74  | C    |
| 24  | AX    | 75  | C    |
| 25  | AY    | 8   | U    |
| 25  | AY    | 11  | C    |
| 25  | AY    | 15  | G    |
| 25  | AY    | 16  | C    |
| 25  | AY    | 17  | G    |
| 25  | AY    | 18  | G    |
| 25  | AY    | 20  | A    |
| 25  | AY    | 21  | A    |
| 25  | AY    | 36  | A    |
| 25  | AY    | 38  | U    |
| 25  | AY    | 39  | C    |
| 25  | AY    | 42  | G    |
| 25  | AY    | 44  | U    |
| 25  | AY    | 45  | U    |
| 25  | AY    | 46  | U    |
| 25  | AY    | 48  | C    |
| 25  | AY    | 50  | A    |
| 25  | AY    | 57  | A    |
| 25  | AY    | 58  | A    |
| 25  | AY    | 60  | C    |
| 25  | AY    | 61  | C    |
| 25  | AY    | 69  | C    |
| 25  | AY    | 73  | C    |
| 27  | BA    | 13  | A    |
| 27  | BA    | 26  | G    |
| 27  | BA    | 28  | A    |
| 27  | BA    | 33  | U    |
| 27  | BA    | 34  | C    |
| 27  | BA    | 45  | C    |
| 27  | BA    | 49  | A    |
| 27  | BA    | 50  | U    |
| 27  | BA    | 55  | G    |
| 27  | BA    | 62  | C    |
| 27  | BA    | 64  | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 27         | BA           | 69         | C           |
| 27         | BA           | 71         | A           |
| 27         | BA           | 72         | U           |
| 27         | BA           | 74         | A           |
| 27         | BA           | 75         | G           |
| 27         | BA           | 84         | A           |
| 27         | BA           | 85         | G           |
| 27         | BA           | 88         | G           |
| 27         | BA           | 90         | U           |
| 27         | BA           | 92         | A           |
| 27         | BA           | 93         | G           |
| 27         | BA           | 94         | C           |
| 27         | BA           | 99         | U           |
| 27         | BA           | 100        | G           |
| 27         | BA           | 102        | G           |
| 27         | BA           | 113        | G           |
| 27         | BA           | 117        | G           |
| 27         | BA           | 118        | A           |
| 27         | BA           | 119        | A           |
| 27         | BA           | 120        | U           |
| 27         | BA           | 121        | G           |
| 27         | BA           | 122        | G           |
| 27         | BA           | 125        | G           |
| 27         | BA           | 126        | A           |
| 27         | BA           | 128        | C           |
| 27         | BA           | 129        | C           |
| 27         | BA           | 131        | G           |
| 27         | BA           | 139(A)     | G           |
| 27         | BA           | 141        | A           |
| 27         | BA           | 148        | C           |
| 27         | BA           | 154        | G           |
| 27         | BA           | 154(A)     | C           |
| 27         | BA           | 157        | U           |
| 27         | BA           | 158        | U           |
| 27         | BA           | 174        | C           |
| 27         | BA           | 175        | G           |
| 27         | BA           | 178        | G           |
| 27         | BA           | 182        | A           |
| 27         | BA           | 196        | A           |
| 27         | BA           | 197        | A           |
| 27         | BA           | 199        | A           |
| 27         | BA           | 200        | U           |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 27  | BA    | 201    | C    |
| 27  | BA    | 204    | A    |
| 27  | BA    | 205    | G    |
| 27  | BA    | 206    | U    |
| 27  | BA    | 215    | G    |
| 27  | BA    | 216    | A    |
| 27  | BA    | 221    | A    |
| 27  | BA    | 222    | A    |
| 27  | BA    | 226    | G    |
| 27  | BA    | 227    | A    |
| 27  | BA    | 228    | A    |
| 27  | BA    | 229    | A    |
| 27  | BA    | 230    | U    |
| 27  | BA    | 232    | G    |
| 27  | BA    | 233    | A    |
| 27  | BA    | 239    | U    |
| 27  | BA    | 248    | G    |
| 27  | BA    | 261    | G    |
| 27  | BA    | 264    | C    |
| 27  | BA    | 266    | G    |
| 27  | BA    | 271(A) | A    |
| 27  | BA    | 271(G) | C    |
| 27  | BA    | 271(H) | G    |
| 27  | BA    | 271(J) | C    |
| 27  | BA    | 271(K) | U    |
| 27  | BA    | 271(L) | U    |
| 27  | BA    | 271(P) | C    |
| 27  | BA    | 271(T) | C    |
| 27  | BA    | 271(W) | G    |
| 27  | BA    | 271(Y) | U    |
| 27  | BA    | 271(Z) | C    |
| 27  | BA    | 272    | G    |
| 27  | BA    | 272(H) | C    |
| 27  | BA    | 272(J) | C    |
| 27  | BA    | 275    | G    |
| 27  | BA    | 283    | A    |
| 27  | BA    | 284    | U    |
| 27  | BA    | 286    | C    |
| 27  | BA    | 287    | C    |
| 27  | BA    | 295    | G    |
| 27  | BA    | 301    | G    |
| 27  | BA    | 302    | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 27  | BA    | 305    | U    |
| 27  | BA    | 310    | A    |
| 27  | BA    | 311    | A    |
| 27  | BA    | 316    | C    |
| 27  | BA    | 322    | A    |
| 27  | BA    | 323    | G    |
| 27  | BA    | 329    | G    |
| 27  | BA    | 330    | A    |
| 27  | BA    | 335    | C    |
| 27  | BA    | 341    | G    |
| 27  | BA    | 346    | A    |
| 27  | BA    | 352    | G    |
| 27  | BA    | 356    | G    |
| 27  | BA    | 358    | U    |
| 27  | BA    | 362    | U    |
| 27  | BA    | 363(B) | G    |
| 27  | BA    | 363(E) | U    |
| 27  | BA    | 363(F) | A    |
| 27  | BA    | 365    | C    |
| 27  | BA    | 371    | A    |
| 27  | BA    | 372    | G    |
| 27  | BA    | 386    | G    |
| 27  | BA    | 387    | U    |
| 27  | BA    | 391    | G    |
| 27  | BA    | 392    | C    |
| 27  | BA    | 394    | A    |
| 27  | BA    | 396    | G    |
| 27  | BA    | 398    | G    |
| 27  | BA    | 400    | G    |
| 27  | BA    | 402    | A    |
| 27  | BA    | 405    | U    |
| 27  | BA    | 406    | G    |
| 27  | BA    | 411    | G    |
| 27  | BA    | 412    | A    |
| 27  | BA    | 416    | C    |
| 27  | BA    | 421    | U    |
| 27  | BA    | 422    | A    |
| 27  | BA    | 428    | A    |
| 27  | BA    | 434    | U    |
| 27  | BA    | 435    | C    |
| 27  | BA    | 441    | U    |
| 27  | BA    | 443    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | BA    | 448 | U    |
| 27  | BA    | 455 | C    |
| 27  | BA    | 456 | C    |
| 27  | BA    | 457 | A    |
| 27  | BA    | 470 | A    |
| 27  | BA    | 471 | A    |
| 27  | BA    | 473 | G    |
| 27  | BA    | 475 | U    |
| 27  | BA    | 479 | A    |
| 27  | BA    | 480 | A    |
| 27  | BA    | 481 | G    |
| 27  | BA    | 482 | A    |
| 27  | BA    | 494 | G    |
| 27  | BA    | 503 | A    |
| 27  | BA    | 504 | U    |
| 27  | BA    | 505 | A    |
| 27  | BA    | 508 | G    |
| 27  | BA    | 509 | C    |
| 27  | BA    | 510 | C    |
| 27  | BA    | 512 | G    |
| 27  | BA    | 525 | U    |
| 27  | BA    | 528 | A    |
| 27  | BA    | 530 | G    |
| 27  | BA    | 531 | C    |
| 27  | BA    | 532 | A    |
| 27  | BA    | 543 | C    |
| 27  | BA    | 548 | A    |
| 27  | BA    | 549 | G    |
| 27  | BA    | 551 | G    |
| 27  | BA    | 556 | G    |
| 27  | BA    | 561 | G    |
| 27  | BA    | 562 | U    |
| 27  | BA    | 563 | G    |
| 27  | BA    | 571 | A    |
| 27  | BA    | 572 | A    |
| 27  | BA    | 573 | G    |
| 27  | BA    | 574 | C    |
| 27  | BA    | 575 | A    |
| 27  | BA    | 588 | U    |
| 27  | BA    | 603 | A    |
| 27  | BA    | 604 | G    |
| 27  | BA    | 607 | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 27  | BA    | 610    | G    |
| 27  | BA    | 614    | U    |
| 27  | BA    | 614(B) | G    |
| 27  | BA    | 615    | G    |
| 27  | BA    | 620    | G    |
| 27  | BA    | 621    | A    |
| 27  | BA    | 622    | G    |
| 27  | BA    | 627    | A    |
| 27  | BA    | 628    | G    |
| 27  | BA    | 634    | C    |
| 27  | BA    | 637    | A    |
| 27  | BA    | 638    | G    |
| 27  | BA    | 645    | C    |
| 27  | BA    | 646    | A    |
| 27  | BA    | 652    | C    |
| 27  | BA    | 657    | U    |
| 27  | BA    | 668    | G    |
| 27  | BA    | 669    | G    |
| 27  | BA    | 670    | A    |
| 27  | BA    | 671    | C    |
| 27  | BA    | 686    | G    |
| 27  | BA    | 708    | C    |
| 27  | BA    | 717    | G    |
| 27  | BA    | 721    | C    |
| 27  | BA    | 722    | A    |
| 27  | BA    | 726    | G    |
| 27  | BA    | 729    | G    |
| 27  | BA    | 730    | C    |
| 27  | BA    | 740    | U    |
| 27  | BA    | 747    | U    |
| 27  | BA    | 748    | G    |
| 27  | BA    | 753    | C    |
| 27  | BA    | 754    | C    |
| 27  | BA    | 755    | C    |
| 27  | BA    | 762    | U    |
| 27  | BA    | 763    | G    |
| 27  | BA    | 764    | A    |
| 27  | BA    | 776    | G    |
| 27  | BA    | 779    | U    |
| 27  | BA    | 782    | A    |
| 27  | BA    | 784    | A    |
| 27  | BA    | 785    | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 27         | BA           | 790        | C           |
| 27         | BA           | 791        | C           |
| 27         | BA           | 792        | G           |
| 27         | BA           | 793        | A           |
| 27         | BA           | 805        | G           |
| 27         | BA           | 806        | C           |
| 27         | BA           | 812        | C           |
| 27         | BA           | 819        | A           |
| 27         | BA           | 826        | U           |
| 27         | BA           | 827        | U           |
| 27         | BA           | 828        | U           |
| 27         | BA           | 830        | G           |
| 27         | BA           | 841        | A           |
| 27         | BA           | 845        | G           |
| 27         | BA           | 846        | C           |
| 27         | BA           | 848        | G           |
| 27         | BA           | 857        | C           |
| 27         | BA           | 859        | G           |
| 27         | BA           | 866        | A           |
| 27         | BA           | 888        | C           |
| 27         | BA           | 890        | A           |
| 27         | BA           | 896        | A           |
| 27         | BA           | 897        | C           |
| 27         | BA           | 900        | A           |
| 27         | BA           | 904        | C           |
| 27         | BA           | 907        | U           |
| 27         | BA           | 910        | A           |
| 27         | BA           | 914        | C           |
| 27         | BA           | 917        | A           |
| 27         | BA           | 932        | G           |
| 27         | BA           | 933        | A           |
| 27         | BA           | 941        | A           |
| 27         | BA           | 946        | G           |
| 27         | BA           | 952        | G           |
| 27         | BA           | 958        | U           |
| 27         | BA           | 959        | A           |
| 27         | BA           | 961        | C           |
| 27         | BA           | 964        | C           |
| 27         | BA           | 974        | G           |
| 27         | BA           | 975        | C           |
| 27         | BA           | 983        | A           |
| 27         | BA           | 985        | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 27         | BA           | 990        | A           |
| 27         | BA           | 991        | C           |
| 27         | BA           | 994        | C           |
| 27         | BA           | 996        | A           |
| 27         | BA           | 997        | G           |
| 27         | BA           | 1005       | C           |
| 27         | BA           | 1008       | C           |
| 27         | BA           | 1009       | A           |
| 27         | BA           | 1012       | U           |
| 27         | BA           | 1013       | C           |
| 27         | BA           | 1017       | G           |
| 27         | BA           | 1020       | A           |
| 27         | BA           | 1021       | A           |
| 27         | BA           | 1022       | G           |
| 27         | BA           | 1023       | U           |
| 27         | BA           | 1024       | G           |
| 27         | BA           | 1025       | G           |
| 27         | BA           | 1026       | U           |
| 27         | BA           | 1031       | G           |
| 27         | BA           | 1033       | U           |
| 27         | BA           | 1034       | G           |
| 27         | BA           | 1035       | U           |
| 27         | BA           | 1042       | G           |
| 27         | BA           | 1043       | C           |
| 27         | BA           | 1044       | G           |
| 27         | BA           | 1045       | A           |
| 27         | BA           | 1046       | A           |
| 27         | BA           | 1047       | G           |
| 27         | BA           | 1049       | C           |
| 27         | BA           | 1050       | A           |
| 27         | BA           | 1051       | G           |
| 27         | BA           | 1052       | C           |
| 27         | BA           | 1053       | C           |
| 27         | BA           | 1054       | A           |
| 27         | BA           | 1110       | G           |
| 27         | BA           | 1111       | A           |
| 27         | BA           | 1112       | G           |
| 27         | BA           | 1113       | U           |
| 27         | BA           | 1115       | G           |
| 27         | BA           | 1122       | G           |
| 27         | BA           | 1126       | A           |
| 27         | BA           | 1127       | A           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | BA    | 1128    | A    |
| 27  | BA    | 1129    | A    |
| 27  | BA    | 1130    | U    |
| 27  | BA    | 1131    | G    |
| 27  | BA    | 1132    | A    |
| 27  | BA    | 1135    | C    |
| 27  | BA    | 1136    | G    |
| 27  | BA    | 1140    | C    |
| 27  | BA    | 1141    | U    |
| 27  | BA    | 1142    | U    |
| 27  | BA    | 1142(A) | A    |
| 27  | BA    | 1143    | A    |
| 27  | BA    | 1155    | A    |
| 27  | BA    | 1170    | G    |
| 27  | BA    | 1171    | G    |
| 27  | BA    | 1173    | G    |
| 27  | BA    | 1174    | A    |
| 27  | BA    | 1175    | U    |
| 27  | BA    | 1176    | G    |
| 27  | BA    | 1177    | A    |
| 27  | BA    | 1178    | C    |
| 27  | BA    | 1179    | C    |
| 27  | BA    | 1180    | C    |
| 27  | BA    | 1186    | G    |
| 27  | BA    | 1190    | G    |
| 27  | BA    | 1193    | G    |
| 27  | BA    | 1195    | G    |
| 27  | BA    | 1204    | A    |
| 27  | BA    | 1205    | U    |
| 27  | BA    | 1211    | U    |
| 27  | BA    | 1212    | G    |
| 27  | BA    | 1213    | A    |
| 27  | BA    | 1214    | A    |
| 27  | BA    | 1220    | A    |
| 27  | BA    | 1221    | C    |
| 27  | BA    | 1224    | C    |
| 27  | BA    | 1226    | A    |
| 27  | BA    | 1230    | C    |
| 27  | BA    | 1233    | C    |
| 27  | BA    | 1236    | G    |
| 27  | BA    | 1237    | A    |
| 27  | BA    | 1248    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | BA    | 1249 | U    |
| 27  | BA    | 1250 | G    |
| 27  | BA    | 1251 | C    |
| 27  | BA    | 1253 | A    |
| 27  | BA    | 1256 | G    |
| 27  | BA    | 1265 | A    |
| 27  | BA    | 1271 | G    |
| 27  | BA    | 1272 | A    |
| 27  | BA    | 1273 | U    |
| 27  | BA    | 1274 | A    |
| 27  | BA    | 1276 | A    |
| 27  | BA    | 1281 | G    |
| 27  | BA    | 1287 | A    |
| 27  | BA    | 1289 | C    |
| 27  | BA    | 1294 | U    |
| 27  | BA    | 1300 | U    |
| 27  | BA    | 1301 | A    |
| 27  | BA    | 1314 | C    |
| 27  | BA    | 1319 | G    |
| 27  | BA    | 1320 | C    |
| 27  | BA    | 1321 | A    |
| 27  | BA    | 1322 | A    |
| 27  | BA    | 1328 | G    |
| 27  | BA    | 1332 | G    |
| 27  | BA    | 1338 | G    |
| 27  | BA    | 1341 | U    |
| 27  | BA    | 1349 | A    |
| 27  | BA    | 1352 | U    |
| 27  | BA    | 1354 | A    |
| 27  | BA    | 1359 | A    |
| 27  | BA    | 1360 | A    |
| 27  | BA    | 1365 | A    |
| 27  | BA    | 1368 | G    |
| 27  | BA    | 1379 | A    |
| 27  | BA    | 1380 | G    |
| 27  | BA    | 1384 | A    |
| 27  | BA    | 1386 | C    |
| 27  | BA    | 1406 | U    |
| 27  | BA    | 1407 | C    |
| 27  | BA    | 1415 | U    |
| 27  | BA    | 1416 | G    |
| 27  | BA    | 1419 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | BA    | 1420    | U    |
| 27  | BA    | 1427    | A    |
| 27  | BA    | 1428    | C    |
| 27  | BA    | 1429    | G    |
| 27  | BA    | 1430    | C    |
| 27  | BA    | 1437    | C    |
| 27  | BA    | 1445    | A    |
| 27  | BA    | 1445(A) | C    |
| 27  | BA    | 1449    | A    |
| 27  | BA    | 1450    | G    |
| 27  | BA    | 1455    | G    |
| 27  | BA    | 1459    | G    |
| 27  | BA    | 1460    | A    |
| 27  | BA    | 1461    | G    |
| 27  | BA    | 1467    | C    |
| 27  | BA    | 1471    | A    |
| 27  | BA    | 1482    | G    |
| 27  | BA    | 1485    | G    |
| 27  | BA    | 1490    | A    |
| 27  | BA    | 1491    | G    |
| 27  | BA    | 1493    | C    |
| 27  | BA    | 1494    | A    |
| 27  | BA    | 1495    | A    |
| 27  | BA    | 1497    | U    |
| 27  | BA    | 1498    | C    |
| 27  | BA    | 1500    | G    |
| 27  | BA    | 1501    | C    |
| 27  | BA    | 1502    | C    |
| 27  | BA    | 1505    | C    |
| 27  | BA    | 1506    | C    |
| 27  | BA    | 1509    | C    |
| 27  | BA    | 1509(A) | A    |
| 27  | BA    | 1518    | U    |
| 27  | BA    | 1525    | G    |
| 27  | BA    | 1547    | C    |
| 27  | BA    | 1554    | A    |
| 27  | BA    | 1558    | A    |
| 27  | BA    | 1559    | G    |
| 27  | BA    | 1566    | A    |
| 27  | BA    | 1568    | G    |
| 27  | BA    | 1569    | A    |
| 27  | BA    | 1578    | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | BA    | 1579    | A    |
| 27  | BA    | 1584    | C    |
| 27  | BA    | 1586    | A    |
| 27  | BA    | 1588    | C    |
| 27  | BA    | 1594    | G    |
| 27  | BA    | 1595    | G    |
| 27  | BA    | 1597    | A    |
| 27  | BA    | 1598    | C    |
| 27  | BA    | 1603    | A    |
| 27  | BA    | 1604    | C    |
| 27  | BA    | 1608    | A    |
| 27  | BA    | 1609    | A    |
| 27  | BA    | 1610    | A    |
| 27  | BA    | 1615    | C    |
| 27  | BA    | 1616    | A    |
| 27  | BA    | 1617    | C    |
| 27  | BA    | 1618    | A    |
| 27  | BA    | 1622    | G    |
| 27  | BA    | 1635    | G    |
| 27  | BA    | 1636    | C    |
| 27  | BA    | 1640    | C    |
| 27  | BA    | 1648    | C    |
| 27  | BA    | 1651    | G    |
| 27  | BA    | 1670    | C    |
| 27  | BA    | 1674    | G    |
| 27  | BA    | 1675    | C    |
| 27  | BA    | 1681    | G    |
| 27  | BA    | 1682    | G    |
| 27  | BA    | 1686    | C    |
| 27  | BA    | 1699    | G    |
| 27  | BA    | 1700    | A    |
| 27  | BA    | 1703    | G    |
| 27  | BA    | 1707    | G    |
| 27  | BA    | 1717    | G    |
| 27  | BA    | 1718    | G    |
| 27  | BA    | 1721    | G    |
| 27  | BA    | 1722    | A    |
| 27  | BA    | 1739    | U    |
| 27  | BA    | 1740    | G    |
| 27  | BA    | 1742    | G    |
| 27  | BA    | 1745(A) | C    |
| 27  | BA    | 1748    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | BA    | 1754 | C    |
| 27  | BA    | 1758 | G    |
| 27  | BA    | 1759 | A    |
| 27  | BA    | 1763 | G    |
| 27  | BA    | 1764 | G    |
| 27  | BA    | 1771 | C    |
| 27  | BA    | 1773 | A    |
| 27  | BA    | 1776 | G    |
| 27  | BA    | 1780 | A    |
| 27  | BA    | 1781 | C    |
| 27  | BA    | 1785 | A    |
| 27  | BA    | 1788 | C    |
| 27  | BA    | 1791 | A    |
| 27  | BA    | 1799 | G    |
| 27  | BA    | 1800 | C    |
| 27  | BA    | 1802 | A    |
| 27  | BA    | 1815 | A    |
| 27  | BA    | 1816 | G    |
| 27  | BA    | 1820 | U    |
| 27  | BA    | 1829 | A    |
| 27  | BA    | 1835 | G    |
| 27  | BA    | 1838 | C    |
| 27  | BA    | 1839 | G    |
| 27  | BA    | 1840 | G    |
| 27  | BA    | 1847 | A    |
| 27  | BA    | 1848 | A    |
| 27  | BA    | 1858 | G    |
| 27  | BA    | 1865 | G    |
| 27  | BA    | 1877 | A    |
| 27  | BA    | 1878 | G    |
| 27  | BA    | 1880 | C    |
| 27  | BA    | 1882 | C    |
| 27  | BA    | 1885 | A    |
| 27  | BA    | 1888 | G    |
| 27  | BA    | 1889 | A    |
| 27  | BA    | 1892 | C    |
| 27  | BA    | 1900 | A    |
| 27  | BA    | 1905 | C    |
| 27  | BA    | 1906 | G    |
| 27  | BA    | 1912 | A    |
| 27  | BA    | 1913 | A    |
| 27  | BA    | 1915 | U    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 27         | BA           | 1919       | A           |
| 27         | BA           | 1926       | U           |
| 27         | BA           | 1930       | G           |
| 27         | BA           | 1931       | U           |
| 27         | BA           | 1936       | A           |
| 27         | BA           | 1937       | A           |
| 27         | BA           | 1938       | A           |
| 27         | BA           | 1940       | U           |
| 27         | BA           | 1946       | U           |
| 27         | BA           | 1954       | G           |
| 27         | BA           | 1955       | U           |
| 27         | BA           | 1963       | U           |
| 27         | BA           | 1964       | G           |
| 27         | BA           | 1965       | C           |
| 27         | BA           | 1967       | C           |
| 27         | BA           | 1969       | A           |
| 27         | BA           | 1970       | A           |
| 27         | BA           | 1971       | A           |
| 27         | BA           | 1972       | A           |
| 27         | BA           | 1981       | A           |
| 27         | BA           | 1982       | C           |
| 27         | BA           | 1991       | U           |
| 27         | BA           | 1993       | U           |
| 27         | BA           | 1996       | C           |
| 27         | BA           | 1997       | G           |
| 27         | BA           | 2006       | C           |
| 27         | BA           | 2019       | A           |
| 27         | BA           | 2020       | A           |
| 27         | BA           | 2021       | C           |
| 27         | BA           | 2022       | U           |
| 27         | BA           | 2023       | G           |
| 27         | BA           | 2026       | C           |
| 27         | BA           | 2030       | A           |
| 27         | BA           | 2031       | A           |
| 27         | BA           | 2032       | G           |
| 27         | BA           | 2033       | A           |
| 27         | BA           | 2036       | C           |
| 27         | BA           | 2037       | G           |
| 27         | BA           | 2041       | U           |
| 27         | BA           | 2043       | C           |
| 27         | BA           | 2048       | G           |
| 27         | BA           | 2049       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | BA    | 2051 | A    |
| 27  | BA    | 2052 | G    |
| 27  | BA    | 2055 | C    |
| 27  | BA    | 2056 | G    |
| 27  | BA    | 2058 | A    |
| 27  | BA    | 2059 | A    |
| 27  | BA    | 2060 | A    |
| 27  | BA    | 2061 | G    |
| 27  | BA    | 2062 | A    |
| 27  | BA    | 2068 | U    |
| 27  | BA    | 2069 | G    |
| 27  | BA    | 2092 | U    |
| 27  | BA    | 2093 | G    |
| 27  | BA    | 2099 | U    |
| 27  | BA    | 2100 | G    |
| 27  | BA    | 2101 | G    |
| 27  | BA    | 2103 | C    |
| 27  | BA    | 2104 | G    |
| 27  | BA    | 2110 | G    |
| 27  | BA    | 2111 | C    |
| 27  | BA    | 2112 | G    |
| 27  | BA    | 2113 | U    |
| 27  | BA    | 2116 | G    |
| 27  | BA    | 2117 | A    |
| 27  | BA    | 2118 | U    |
| 27  | BA    | 2119 | A    |
| 27  | BA    | 2120 | G    |
| 27  | BA    | 2121 | G    |
| 27  | BA    | 2126 | A    |
| 27  | BA    | 2127 | G    |
| 27  | BA    | 2128 | C    |
| 27  | BA    | 2131 | G    |
| 27  | BA    | 2132 | U    |
| 27  | BA    | 2133 | G    |
| 27  | BA    | 2136 | C    |
| 27  | BA    | 2146 | C    |
| 27  | BA    | 2147 | G    |
| 27  | BA    | 2157 | G    |
| 27  | BA    | 2159 | G    |
| 27  | BA    | 2160 | G    |
| 27  | BA    | 2172 | U    |
| 27  | BA    | 2173 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | BA    | 2174 | C    |
| 27  | BA    | 2175 | C    |
| 27  | BA    | 2178 | C    |
| 27  | BA    | 2185 | C    |
| 27  | BA    | 2187 | G    |
| 27  | BA    | 2190 | G    |
| 27  | BA    | 2192 | G    |
| 27  | BA    | 2193 | G    |
| 27  | BA    | 2198 | A    |
| 27  | BA    | 2199 | A    |
| 27  | BA    | 2200 | C    |
| 27  | BA    | 2201 | C    |
| 27  | BA    | 2207 | G    |
| 27  | BA    | 2208 | A    |
| 27  | BA    | 2218 | U    |
| 27  | BA    | 2219 | G    |
| 27  | BA    | 2226 | C    |
| 27  | BA    | 2238 | G    |
| 27  | BA    | 2239 | G    |
| 27  | BA    | 2240 | C    |
| 27  | BA    | 2250 | G    |
| 27  | BA    | 2251 | G    |
| 27  | BA    | 2252 | G    |
| 27  | BA    | 2266 | A    |
| 27  | BA    | 2267 | A    |
| 27  | BA    | 2268 | A    |
| 27  | BA    | 2273 | A    |
| 27  | BA    | 2275 | C    |
| 27  | BA    | 2283 | C    |
| 27  | BA    | 2287 | A    |
| 27  | BA    | 2288 | A    |
| 27  | BA    | 2290 | G    |
| 27  | BA    | 2293 | C    |
| 27  | BA    | 2297 | C    |
| 27  | BA    | 2305 | A    |
| 27  | BA    | 2306 | C    |
| 27  | BA    | 2307 | G    |
| 27  | BA    | 2308 | G    |
| 27  | BA    | 2309 | A    |
| 27  | BA    | 2310 | A    |
| 27  | BA    | 2311 | A    |
| 27  | BA    | 2312 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | BA    | 2314 | C    |
| 27  | BA    | 2318 | G    |
| 27  | BA    | 2319 | G    |
| 27  | BA    | 2320 | A    |
| 27  | BA    | 2321 | G    |
| 27  | BA    | 2325 | G    |
| 27  | BA    | 2326 | C    |
| 27  | BA    | 2327 | A    |
| 27  | BA    | 2329 | G    |
| 27  | BA    | 2334 | G    |
| 27  | BA    | 2335 | A    |
| 27  | BA    | 2336 | A    |
| 27  | BA    | 2342 | C    |
| 27  | BA    | 2345 | G    |
| 27  | BA    | 2347 | C    |
| 27  | BA    | 2349 | G    |
| 27  | BA    | 2350 | C    |
| 27  | BA    | 2358 | G    |
| 27  | BA    | 2383 | G    |
| 27  | BA    | 2384 | G    |
| 27  | BA    | 2385 | C    |
| 27  | BA    | 2387 | U    |
| 27  | BA    | 2388 | A    |
| 27  | BA    | 2391 | G    |
| 27  | BA    | 2392 | A    |
| 27  | BA    | 2399 | G    |
| 27  | BA    | 2400 | G    |
| 27  | BA    | 2402 | C    |
| 27  | BA    | 2407 | G    |
| 27  | BA    | 2411 | A    |
| 27  | BA    | 2414 | G    |
| 27  | BA    | 2424 | C    |
| 27  | BA    | 2425 | A    |
| 27  | BA    | 2427 | C    |
| 27  | BA    | 2429 | G    |
| 27  | BA    | 2430 | A    |
| 27  | BA    | 2435 | A    |
| 27  | BA    | 2439 | A    |
| 27  | BA    | 2440 | C    |
| 27  | BA    | 2441 | C    |
| 27  | BA    | 2448 | A    |
| 27  | BA    | 2459 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | BA    | 2469 | A    |
| 27  | BA    | 2470 | G    |
| 27  | BA    | 2474 | C    |
| 27  | BA    | 2476 | A    |
| 27  | BA    | 2477 | C    |
| 27  | BA    | 2478 | A    |
| 27  | BA    | 2482 | G    |
| 27  | BA    | 2484 | G    |
| 27  | BA    | 2486 | G    |
| 27  | BA    | 2487 | G    |
| 27  | BA    | 2491 | U    |
| 27  | BA    | 2495 | G    |
| 27  | BA    | 2502 | G    |
| 27  | BA    | 2503 | A    |
| 27  | BA    | 2504 | U    |
| 27  | BA    | 2505 | G    |
| 27  | BA    | 2506 | U    |
| 27  | BA    | 2513 | G    |
| 27  | BA    | 2518 | A    |
| 27  | BA    | 2520 | C    |
| 27  | BA    | 2523 | G    |
| 27  | BA    | 2525 | G    |
| 27  | BA    | 2529 | G    |
| 27  | BA    | 2534 | A    |
| 27  | BA    | 2535 | G    |
| 27  | BA    | 2543 | G    |
| 27  | BA    | 2546 | U    |
| 27  | BA    | 2550 | G    |
| 27  | BA    | 2554 | U    |
| 27  | BA    | 2559 | C    |
| 27  | BA    | 2566 | A    |
| 27  | BA    | 2567 | G    |
| 27  | BA    | 2573 | C    |
| 27  | BA    | 2577 | A    |
| 27  | BA    | 2582 | G    |
| 27  | BA    | 2586 | C    |
| 27  | BA    | 2602 | A    |
| 27  | BA    | 2610 | C    |
| 27  | BA    | 2611 | U    |
| 27  | BA    | 2612 | C    |
| 27  | BA    | 2614 | A    |
| 27  | BA    | 2615 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | BA    | 2630    | G    |
| 27  | BA    | 2639    | A    |
| 27  | BA    | 2646    | C    |
| 27  | BA    | 2654    | A    |
| 27  | BA    | 2655    | G    |
| 27  | BA    | 2656    | U    |
| 27  | BA    | 2670    | A    |
| 27  | BA    | 2682    | U    |
| 27  | BA    | 2690    | C    |
| 27  | BA    | 2691    | C    |
| 27  | BA    | 2694    | G    |
| 27  | BA    | 2702    | U    |
| 27  | BA    | 2703    | C    |
| 27  | BA    | 2707    | G    |
| 27  | BA    | 2712    | U    |
| 27  | BA    | 2712(A) | A    |
| 27  | BA    | 2713    | A    |
| 27  | BA    | 2725    | A    |
| 27  | BA    | 2726    | U    |
| 27  | BA    | 2727    | G    |
| 27  | BA    | 2729    | G    |
| 27  | BA    | 2732    | G    |
| 27  | BA    | 2733    | A    |
| 27  | BA    | 2739    | U    |
| 27  | BA    | 2744    | G    |
| 27  | BA    | 2751    | G    |
| 27  | BA    | 2752    | C    |
| 27  | BA    | 2757    | A    |
| 27  | BA    | 2761    | G    |
| 27  | BA    | 2764    | A    |
| 27  | BA    | 2765    | A    |
| 27  | BA    | 2777    | G    |
| 27  | BA    | 2778    | A    |
| 27  | BA    | 2779    | U    |
| 27  | BA    | 2789    | C    |
| 27  | BA    | 2790    | A    |
| 27  | BA    | 2791    | C    |
| 27  | BA    | 2792    | G    |
| 27  | BA    | 2793    | G    |
| 27  | BA    | 2794    | C    |
| 27  | BA    | 2796    | U    |
| 27  | BA    | 2799    | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | BA    | 2801    | A    |
| 27  | BA    | 2801(A) | A    |
| 27  | BA    | 2802    | G    |
| 27  | BA    | 2803    | C    |
| 27  | BA    | 2804    | C    |
| 27  | BA    | 2807    | G    |
| 27  | BA    | 2808    | U    |
| 27  | BA    | 2813    | A    |
| 27  | BA    | 2817    | G    |
| 27  | BA    | 2818    | G    |
| 27  | BA    | 2820    | A    |
| 27  | BA    | 2821    | A    |
| 27  | BA    | 2833    | G    |
| 27  | BA    | 2834    | G    |
| 27  | BA    | 2835    | A    |
| 27  | BA    | 2836    | U    |
| 27  | BA    | 2848    | G    |
| 27  | BA    | 2849    | U    |
| 27  | BA    | 2857    | G    |
| 27  | BA    | 2864    | G    |
| 27  | BA    | 2868    | A    |
| 27  | BA    | 2872    | G    |
| 27  | BA    | 2874    | C    |
| 27  | BA    | 2875    | C    |
| 27  | BA    | 2876    | G    |
| 27  | BA    | 2877    | G    |
| 27  | BA    | 2879    | C    |
| 27  | BA    | 2880    | C    |
| 27  | BA    | 2893    | G    |
| 27  | BA    | 2894    | G    |
| 27  | BA    | 2895    | U    |
| 28  | BB    | 2       | C    |
| 28  | BB    | 8       | U    |
| 28  | BB    | 12      | C    |
| 28  | BB    | 13      | A    |
| 28  | BB    | 14      | U    |
| 28  | BB    | 15      | A    |
| 28  | BB    | 24      | G    |
| 28  | BB    | 25      | A    |
| 28  | BB    | 26      | A    |
| 28  | BB    | 32      | C    |
| 28  | BB    | 35      | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 28  | BB    | 42     | C    |
| 28  | BB    | 45     | A    |
| 28  | BB    | 47     | C    |
| 28  | BB    | 52     | A    |
| 28  | BB    | 53     | A    |
| 28  | BB    | 58     | A    |
| 28  | BB    | 67     | G    |
| 28  | BB    | 73     | A    |
| 28  | BB    | 86     | G    |
| 28  | BB    | 88     | C    |
| 28  | BB    | 91     | C    |
| 28  | BB    | 92     | C    |
| 28  | BB    | 95     | C    |
| 28  | BB    | 110    | G    |
| 28  | BB    | 113    | G    |
| 1   | CA    | 8      | A    |
| 1   | CA    | 9      | G    |
| 1   | CA    | 10     | A    |
| 1   | CA    | 14     | U    |
| 1   | CA    | 22     | G    |
| 1   | CA    | 31     | G    |
| 1   | CA    | 32     | A    |
| 1   | CA    | 39     | G    |
| 1   | CA    | 47     | C    |
| 1   | CA    | 48     | C    |
| 1   | CA    | 51     | A    |
| 1   | CA    | 60     | A    |
| 1   | CA    | 61     | G    |
| 1   | CA    | 64     | G    |
| 1   | CA    | 65     | U    |
| 1   | CA    | 66     | G    |
| 1   | CA    | 101    | A    |
| 1   | CA    | 109    | A    |
| 1   | CA    | 110    | C    |
| 1   | CA    | 116    | A    |
| 1   | CA    | 120    | A    |
| 1   | CA    | 121    | C    |
| 1   | CA    | 129(A) | G    |
| 1   | CA    | 130    | A    |
| 1   | CA    | 131    | C    |
| 1   | CA    | 132    | C    |
| 1   | CA    | 137    | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | CA    | 144    | G    |
| 1   | CA    | 146    | G    |
| 1   | CA    | 173    | U    |
| 1   | CA    | 174    | C    |
| 1   | CA    | 182    | U    |
| 1   | CA    | 189(E) | U    |
| 1   | CA    | 194    | C    |
| 1   | CA    | 195    | A    |
| 1   | CA    | 198    | G    |
| 1   | CA    | 200    | G    |
| 1   | CA    | 203    | U    |
| 1   | CA    | 204    | U    |
| 1   | CA    | 216    | G    |
| 1   | CA    | 217    | C    |
| 1   | CA    | 218    | C    |
| 1   | CA    | 219    | C    |
| 1   | CA    | 220    | G    |
| 1   | CA    | 231    | G    |
| 1   | CA    | 241    | C    |
| 1   | CA    | 244    | U    |
| 1   | CA    | 246    | A    |
| 1   | CA    | 247    | G    |
| 1   | CA    | 251    | G    |
| 1   | CA    | 266    | G    |
| 1   | CA    | 267    | C    |
| 1   | CA    | 275    | G    |
| 1   | CA    | 279    | A    |
| 1   | CA    | 280    | C    |
| 1   | CA    | 289    | G    |
| 1   | CA    | 305    | G    |
| 1   | CA    | 306    | G    |
| 1   | CA    | 316    | G    |
| 1   | CA    | 321    | A    |
| 1   | CA    | 328    | C    |
| 1   | CA    | 330    | C    |
| 1   | CA    | 332    | G    |
| 1   | CA    | 342    | C    |
| 1   | CA    | 344    | A    |
| 1   | CA    | 345    | C    |
| 1   | CA    | 346    | G    |
| 1   | CA    | 347    | G    |
| 1   | CA    | 348    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 351 | G    |
| 1   | CA    | 352 | C    |
| 1   | CA    | 353 | A    |
| 1   | CA    | 354 | G    |
| 1   | CA    | 366 | C    |
| 1   | CA    | 367 | U    |
| 1   | CA    | 373 | A    |
| 1   | CA    | 389 | A    |
| 1   | CA    | 397 | A    |
| 1   | CA    | 398 | C    |
| 1   | CA    | 406 | G    |
| 1   | CA    | 411 | A    |
| 1   | CA    | 412 | A    |
| 1   | CA    | 413 | G    |
| 1   | CA    | 414 | A    |
| 1   | CA    | 421 | U    |
| 1   | CA    | 422 | C    |
| 1   | CA    | 423 | G    |
| 1   | CA    | 424 | G    |
| 1   | CA    | 428 | G    |
| 1   | CA    | 429 | U    |
| 1   | CA    | 430 | A    |
| 1   | CA    | 431 | A    |
| 1   | CA    | 435 | C    |
| 1   | CA    | 438 | G    |
| 1   | CA    | 439 | A    |
| 1   | CA    | 442 | C    |
| 1   | CA    | 444 | C    |
| 1   | CA    | 451 | A    |
| 1   | CA    | 452 | A    |
| 1   | CA    | 453 | A    |
| 1   | CA    | 454 | C    |
| 1   | CA    | 455 | C    |
| 1   | CA    | 461 | A    |
| 1   | CA    | 471 | G    |
| 1   | CA    | 472 | A    |
| 1   | CA    | 481 | G    |
| 1   | CA    | 482 | A    |
| 1   | CA    | 484 | G    |
| 1   | CA    | 485 | G    |
| 1   | CA    | 494 | U    |
| 1   | CA    | 495 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 496 | A    |
| 1   | CA    | 498 | U    |
| 1   | CA    | 499 | A    |
| 1   | CA    | 508 | C    |
| 1   | CA    | 509 | A    |
| 1   | CA    | 510 | A    |
| 1   | CA    | 511 | C    |
| 1   | CA    | 512 | U    |
| 1   | CA    | 517 | G    |
| 1   | CA    | 518 | C    |
| 1   | CA    | 527 | G    |
| 1   | CA    | 529 | G    |
| 1   | CA    | 531 | U    |
| 1   | CA    | 532 | A    |
| 1   | CA    | 533 | A    |
| 1   | CA    | 534 | U    |
| 1   | CA    | 547 | A    |
| 1   | CA    | 548 | G    |
| 1   | CA    | 559 | A    |
| 1   | CA    | 560 | U    |
| 1   | CA    | 561 | U    |
| 1   | CA    | 563 | A    |
| 1   | CA    | 564 | C    |
| 1   | CA    | 566 | G    |
| 1   | CA    | 567 | G    |
| 1   | CA    | 572 | A    |
| 1   | CA    | 573 | A    |
| 1   | CA    | 575 | G    |
| 1   | CA    | 576 | G    |
| 1   | CA    | 577 | G    |
| 1   | CA    | 587 | G    |
| 1   | CA    | 596 | C    |
| 1   | CA    | 598 | U    |
| 1   | CA    | 629 | G    |
| 1   | CA    | 630 | G    |
| 1   | CA    | 632 | A    |
| 1   | CA    | 641 | U    |
| 1   | CA    | 642 | A    |
| 1   | CA    | 643 | C    |
| 1   | CA    | 653 | A    |
| 1   | CA    | 654 | G    |
| 1   | CA    | 665 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 666 | G    |
| 1   | CA    | 687 | A    |
| 1   | CA    | 688 | G    |
| 1   | CA    | 701 | C    |
| 1   | CA    | 702 | A    |
| 1   | CA    | 703 | G    |
| 1   | CA    | 720 | C    |
| 1   | CA    | 721 | G    |
| 1   | CA    | 722 | A    |
| 1   | CA    | 729 | A    |
| 1   | CA    | 731 | G    |
| 1   | CA    | 748 | C    |
| 1   | CA    | 749 | C    |
| 1   | CA    | 754 | C    |
| 1   | CA    | 755 | G    |
| 1   | CA    | 774 | G    |
| 1   | CA    | 777 | A    |
| 1   | CA    | 793 | U    |
| 1   | CA    | 794 | A    |
| 1   | CA    | 811 | C    |
| 1   | CA    | 813 | U    |
| 1   | CA    | 815 | A    |
| 1   | CA    | 816 | A    |
| 1   | CA    | 817 | C    |
| 1   | CA    | 818 | G    |
| 1   | CA    | 819 | A    |
| 1   | CA    | 821 | G    |
| 1   | CA    | 827 | U    |
| 1   | CA    | 828 | A    |
| 1   | CA    | 835 | U    |
| 1   | CA    | 839 | U    |
| 1   | CA    | 841 | U    |
| 1   | CA    | 848 | C    |
| 1   | CA    | 851 | G    |
| 1   | CA    | 859 | A    |
| 1   | CA    | 871 | U    |
| 1   | CA    | 874 | G    |
| 1   | CA    | 875 | C    |
| 1   | CA    | 884 | U    |
| 1   | CA    | 885 | G    |
| 1   | CA    | 889 | A    |
| 1   | CA    | 890 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | CA    | 902     | G    |
| 1   | CA    | 914     | A    |
| 1   | CA    | 916     | G    |
| 1   | CA    | 927     | G    |
| 1   | CA    | 934     | C    |
| 1   | CA    | 935     | A    |
| 1   | CA    | 936     | C    |
| 1   | CA    | 960     | U    |
| 1   | CA    | 962     | C    |
| 1   | CA    | 965     | A    |
| 1   | CA    | 966     | G    |
| 1   | CA    | 967     | C    |
| 1   | CA    | 968     | A    |
| 1   | CA    | 969     | A    |
| 1   | CA    | 971     | G    |
| 1   | CA    | 972     | C    |
| 1   | CA    | 974     | A    |
| 1   | CA    | 975     | A    |
| 1   | CA    | 976     | G    |
| 1   | CA    | 977     | A    |
| 1   | CA    | 978     | A    |
| 1   | CA    | 980     | C    |
| 1   | CA    | 981     | U    |
| 1   | CA    | 983     | A    |
| 1   | CA    | 984     | C    |
| 1   | CA    | 985     | C    |
| 1   | CA    | 986     | 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    | 1001(A) | G    |
| 1   | CA    | 1004    | A    |
| 1   | CA    | 1006    | C    |
| 1   | CA    | 1016    | A    |
| 1   | CA    | 1024    | G    |
| 1   | CA    | 1027    | C    |
| 1   | CA    | 1030    | C    |
| 1   | CA    | 1030(A) | G    |
| 1   | CA    | 1030(C) | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1031 | G    |
| 1   | CA    | 1042 | G    |
| 1   | CA    | 1050 | G    |
| 1   | CA    | 1053 | G    |
| 1   | CA    | 1054 | C    |
| 1   | CA    | 1055 | A    |
| 1   | CA    | 1058 | G    |
| 1   | CA    | 1064 | G    |
| 1   | CA    | 1065 | U    |
| 1   | CA    | 1066 | C    |
| 1   | CA    | 1068 | G    |
| 1   | CA    | 1085 | U    |
| 1   | CA    | 1086 | U    |
| 1   | CA    | 1094 | G    |
| 1   | CA    | 1099 | G    |
| 1   | CA    | 1101 | A    |
| 1   | CA    | 1102 | A    |
| 1   | CA    | 1105 | A    |
| 1   | CA    | 1108 | G    |
| 1   | CA    | 1117 | G    |
| 1   | CA    | 1118 | C    |
| 1   | CA    | 1124 | G    |
| 1   | CA    | 1125 | U    |
| 1   | CA    | 1126 | U    |
| 1   | CA    | 1127 | G    |
| 1   | CA    | 1129 | C    |
| 1   | CA    | 1130 | A    |
| 1   | CA    | 1131 | G    |
| 1   | CA    | 1137 | C    |
| 1   | CA    | 1139 | G    |
| 1   | CA    | 1140 | C    |
| 1   | CA    | 1141 | C    |
| 1   | CA    | 1145 | C    |
| 1   | CA    | 1146 | A    |
| 1   | CA    | 1155 | G    |
| 1   | CA    | 1157 | A    |
| 1   | CA    | 1158 | C    |
| 1   | CA    | 1159 | U    |
| 1   | CA    | 1160 | G    |
| 1   | CA    | 1161 | C    |
| 1   | CA    | 1162 | C    |
| 1   | CA    | 1171 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1182 | G    |
| 1   | CA    | 1183 | A    |
| 1   | CA    | 1184 | G    |
| 1   | CA    | 1195 | C    |
| 1   | CA    | 1196 | U    |
| 1   | CA    | 1197 | G    |
| 1   | CA    | 1200 | C    |
| 1   | CA    | 1201 | A    |
| 1   | CA    | 1202 | G    |
| 1   | CA    | 1212 | U    |
| 1   | CA    | 1213 | A    |
| 1   | CA    | 1216 | G    |
| 1   | CA    | 1224 | G    |
| 1   | CA    | 1225 | A    |
| 1   | CA    | 1226 | C    |
| 1   | CA    | 1227 | A    |
| 1   | CA    | 1232 | U    |
| 1   | CA    | 1238 | A    |
| 1   | CA    | 1239 | A    |
| 1   | CA    | 1240 | U    |
| 1   | CA    | 1241 | G    |
| 1   | CA    | 1256 | A    |
| 1   | CA    | 1257 | U    |
| 1   | CA    | 1258 | G    |
| 1   | CA    | 1260 | C    |
| 1   | CA    | 1263 | C    |
| 1   | CA    | 1273 | G    |
| 1   | CA    | 1280 | A    |
| 1   | CA    | 1281 | U    |
| 1   | CA    | 1285 | A    |
| 1   | CA    | 1286 | A    |
| 1   | CA    | 1287 | A    |
| 1   | CA    | 1297 | C    |
| 1   | CA    | 1299 | A    |
| 1   | CA    | 1300 | G    |
| 1   | CA    | 1301 | U    |
| 1   | CA    | 1302 | U    |
| 1   | CA    | 1305 | G    |
| 1   | CA    | 1306 | A    |
| 1   | CA    | 1317 | C    |
| 1   | CA    | 1319 | A    |
| 1   | CA    | 1320 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | CA    | 1322    | C    |
| 1   | CA    | 1323    | G    |
| 1   | CA    | 1331    | G    |
| 1   | CA    | 1334    | G    |
| 1   | CA    | 1336    | C    |
| 1   | CA    | 1338    | G    |
| 1   | CA    | 1347    | G    |
| 1   | CA    | 1363(A) | A    |
| 1   | CA    | 1364    | U    |
| 1   | CA    | 1365    | G    |
| 1   | CA    | 1370    | G    |
| 1   | CA    | 1378    | C    |
| 1   | CA    | 1381    | U    |
| 1   | CA    | 1394    | A    |
| 1   | CA    | 1395    | C    |
| 1   | CA    | 1397    | C    |
| 1   | CA    | 1398    | A    |
| 1   | CA    | 1419    | G    |
| 1   | CA    | 1429    | C    |
| 1   | CA    | 1442    | G    |
| 1   | CA    | 1442(A) | G    |
| 1   | CA    | 1442(B) | A    |
| 1   | CA    | 1443    | G    |
| 1   | CA    | 1444    | C    |
| 1   | CA    | 1447    | A    |
| 1   | CA    | 1452    | C    |
| 1   | CA    | 1456    | G    |
| 1   | CA    | 1492    | A    |
| 1   | CA    | 1498    | U    |
| 1   | CA    | 1499    | A    |
| 1   | CA    | 1502    | A    |
| 1   | CA    | 1503    | A    |
| 1   | CA    | 1504    | G    |
| 1   | CA    | 1505    | G    |
| 1   | CA    | 1506    | U    |
| 1   | CA    | 1507    | A    |
| 1   | CA    | 1517    | G    |
| 1   | CA    | 1519    | A    |
| 1   | CA    | 1520    | G    |
| 1   | CA    | 1521    | G    |
| 1   | CA    | 1525    | G    |
| 1   | CA    | 1528    | U    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | CA    | 1529  | G    |
| 1   | CA    | 1530  | G    |
| 23  | CW    | 8     | U    |
| 23  | CW    | 9     | C    |
| 23  | CW    | 16    | C    |
| 23  | CW    | 17    | G    |
| 23  | CW    | 20    | A    |
| 23  | CW    | 31    | U    |
| 23  | CW    | 36    | A    |
| 23  | CW    | 43    | C    |
| 23  | CW    | 45    | U    |
| 23  | CW    | 48    | C    |
| 23  | CW    | 53    | U    |
| 23  | CW    | 60    | C    |
| 23  | CW    | 71    | A    |
| 23  | CW    | 72    | G    |
| 23  | CW    | 73    | C    |
| 23  | CW    | 74    | C    |
| 24  | CX    | 8     | U    |
| 24  | CX    | 13    | C    |
| 24  | CX    | 17    | C    |
| 24  | CX    | 17(B) | U    |
| 24  | CX    | 19    | G    |
| 24  | CX    | 20    | U    |
| 24  | CX    | 21    | A    |
| 24  | CX    | 47    | U    |
| 24  | CX    | 48    | C    |
| 24  | CX    | 49    | G    |
| 24  | CX    | 51    | C    |
| 24  | CX    | 61    | C    |
| 24  | CX    | 62    | C    |
| 24  | CX    | 63    | G    |
| 24  | CX    | 65    | C    |
| 24  | CX    | 68    | C    |
| 24  | CX    | 73    | A    |
| 24  | CX    | 74    | C    |
| 24  | CX    | 75    | C    |
| 25  | CY    | 8     | U    |
| 25  | CY    | 9     | C    |
| 25  | CY    | 11    | C    |
| 25  | CY    | 12    | C    |
| 25  | CY    | 16    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | CY    | 17  | G    |
| 25  | CY    | 18  | G    |
| 25  | CY    | 20  | A    |
| 25  | CY    | 21  | A    |
| 25  | CY    | 36  | A    |
| 25  | CY    | 38  | U    |
| 25  | CY    | 42  | G    |
| 25  | CY    | 46  | U    |
| 25  | CY    | 47  | C    |
| 25  | CY    | 49  | G    |
| 25  | CY    | 50  | A    |
| 25  | CY    | 55  | C    |
| 25  | CY    | 57  | A    |
| 25  | CY    | 58  | A    |
| 25  | CY    | 60  | C    |
| 25  | CY    | 69  | C    |
| 25  | CY    | 73  | C    |
| 27  | DA    | 19  | C    |
| 27  | DA    | 33  | U    |
| 27  | DA    | 34  | C    |
| 27  | DA    | 35  | G    |
| 27  | DA    | 45  | C    |
| 27  | DA    | 49  | A    |
| 27  | DA    | 50  | U    |
| 27  | DA    | 51  | G    |
| 27  | DA    | 53  | A    |
| 27  | DA    | 61  | G    |
| 27  | DA    | 62  | C    |
| 27  | DA    | 64  | A    |
| 27  | DA    | 69  | C    |
| 27  | DA    | 71  | A    |
| 27  | DA    | 72  | U    |
| 27  | DA    | 73  | A    |
| 27  | DA    | 74  | A    |
| 27  | DA    | 75  | G    |
| 27  | DA    | 83  | G    |
| 27  | DA    | 84  | A    |
| 27  | DA    | 88  | G    |
| 27  | DA    | 90  | U    |
| 27  | DA    | 92  | A    |
| 27  | DA    | 93  | G    |
| 27  | DA    | 94  | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 27  | DA    | 95     | G    |
| 27  | DA    | 99     | U    |
| 27  | DA    | 100    | G    |
| 27  | DA    | 102    | G    |
| 27  | DA    | 113    | G    |
| 27  | DA    | 118    | A    |
| 27  | DA    | 119    | A    |
| 27  | DA    | 120    | U    |
| 27  | DA    | 126    | A    |
| 27  | DA    | 129    | C    |
| 27  | DA    | 139(A) | G    |
| 27  | DA    | 140    | G    |
| 27  | DA    | 141    | A    |
| 27  | DA    | 146    | G    |
| 27  | DA    | 149    | A    |
| 27  | DA    | 150    | C    |
| 27  | DA    | 154    | G    |
| 27  | DA    | 157    | U    |
| 27  | DA    | 158    | U    |
| 27  | DA    | 172    | C    |
| 27  | DA    | 173    | G    |
| 27  | DA    | 175    | G    |
| 27  | DA    | 177    | G    |
| 27  | DA    | 181    | A    |
| 27  | DA    | 182    | A    |
| 27  | DA    | 196    | A    |
| 27  | DA    | 197    | A    |
| 27  | DA    | 199    | A    |
| 27  | DA    | 200    | U    |
| 27  | DA    | 201    | C    |
| 27  | DA    | 204    | A    |
| 27  | DA    | 205    | G    |
| 27  | DA    | 214    | G    |
| 27  | DA    | 216    | A    |
| 27  | DA    | 217    | G    |
| 27  | DA    | 221    | A    |
| 27  | DA    | 222    | A    |
| 27  | DA    | 224    | G    |
| 27  | DA    | 227    | A    |
| 27  | DA    | 228    | A    |
| 27  | DA    | 232    | G    |
| 27  | DA    | 233    | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 27  | DA    | 241    | A    |
| 27  | DA    | 242    | G    |
| 27  | DA    | 248    | G    |
| 27  | DA    | 249    | C    |
| 27  | DA    | 250    | G    |
| 27  | DA    | 252    | G    |
| 27  | DA    | 256    | A    |
| 27  | DA    | 261    | G    |
| 27  | DA    | 266    | G    |
| 27  | DA    | 267    | C    |
| 27  | DA    | 271(J) | C    |
| 27  | DA    | 271(K) | U    |
| 27  | DA    | 271(M) | G    |
| 27  | DA    | 271(O) | C    |
| 27  | DA    | 271(P) | C    |
| 27  | DA    | 271(T) | C    |
| 27  | DA    | 271(Y) | U    |
| 27  | DA    | 271(Z) | C    |
| 27  | DA    | 272    | G    |
| 27  | DA    | 272(C) | G    |
| 27  | DA    | 272(H) | C    |
| 27  | DA    | 272(J) | C    |
| 27  | DA    | 274    | G    |
| 27  | DA    | 275    | G    |
| 27  | DA    | 283    | A    |
| 27  | DA    | 284    | U    |
| 27  | DA    | 285    | C    |
| 27  | DA    | 287    | C    |
| 27  | DA    | 288    | C    |
| 27  | DA    | 289    | A    |
| 27  | DA    | 301    | G    |
| 27  | DA    | 302    | C    |
| 27  | DA    | 310    | A    |
| 27  | DA    | 311    | A    |
| 27  | DA    | 313    | C    |
| 27  | DA    | 314    | A    |
| 27  | DA    | 316    | C    |
| 27  | DA    | 322    | A    |
| 27  | DA    | 323    | G    |
| 27  | DA    | 324    | A    |
| 27  | DA    | 329    | G    |
| 27  | DA    | 330    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 27         | DA           | 332        | A           |
| 27         | DA           | 333        | G           |
| 27         | DA           | 334        | C           |
| 27         | DA           | 338        | G           |
| 27         | DA           | 345        | A           |
| 27         | DA           | 346        | A           |
| 27         | DA           | 352        | G           |
| 27         | DA           | 353        | G           |
| 27         | DA           | 356        | G           |
| 27         | DA           | 358        | U           |
| 27         | DA           | 362        | U           |
| 27         | DA           | 363(B)     | G           |
| 27         | DA           | 363(E)     | U           |
| 27         | DA           | 363(F)     | A           |
| 27         | DA           | 364        | C           |
| 27         | DA           | 371        | A           |
| 27         | DA           | 372        | G           |
| 27         | DA           | 374        | A           |
| 27         | DA           | 387        | U           |
| 27         | DA           | 395        | U           |
| 27         | DA           | 396        | G           |
| 27         | DA           | 404        | C           |
| 27         | DA           | 405        | U           |
| 27         | DA           | 406        | G           |
| 27         | DA           | 411        | G           |
| 27         | DA           | 412        | A           |
| 27         | DA           | 413        | C           |
| 27         | DA           | 416        | C           |
| 27         | DA           | 422        | A           |
| 27         | DA           | 423        | A           |
| 27         | DA           | 428        | A           |
| 27         | DA           | 435        | C           |
| 27         | DA           | 443        | A           |
| 27         | DA           | 444        | C           |
| 27         | DA           | 445        | C           |
| 27         | DA           | 446        | G           |
| 27         | DA           | 447        | A           |
| 27         | DA           | 448        | U           |
| 27         | DA           | 449        | A           |
| 27         | DA           | 455        | C           |
| 27         | DA           | 456        | C           |
| 27         | DA           | 457        | A           |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DA    | 458 | G    |
| 27  | DA    | 460 | A    |
| 27  | DA    | 467 | G    |
| 27  | DA    | 470 | A    |
| 27  | DA    | 473 | G    |
| 27  | DA    | 475 | U    |
| 27  | DA    | 476 | G    |
| 27  | DA    | 478 | A    |
| 27  | DA    | 479 | A    |
| 27  | DA    | 480 | A    |
| 27  | DA    | 481 | G    |
| 27  | DA    | 482 | A    |
| 27  | DA    | 483 | A    |
| 27  | DA    | 492 | A    |
| 27  | DA    | 503 | A    |
| 27  | DA    | 504 | U    |
| 27  | DA    | 505 | A    |
| 27  | DA    | 506 | G    |
| 27  | DA    | 507 | A    |
| 27  | DA    | 509 | C    |
| 27  | DA    | 510 | C    |
| 27  | DA    | 512 | G    |
| 27  | DA    | 515 | A    |
| 27  | DA    | 527 | C    |
| 27  | DA    | 528 | A    |
| 27  | DA    | 530 | G    |
| 27  | DA    | 531 | C    |
| 27  | DA    | 532 | A    |
| 27  | DA    | 533 | G    |
| 27  | DA    | 542 | C    |
| 27  | DA    | 543 | C    |
| 27  | DA    | 548 | A    |
| 27  | DA    | 549 | G    |
| 27  | DA    | 551 | G    |
| 27  | DA    | 555 | U    |
| 27  | DA    | 561 | G    |
| 27  | DA    | 563 | G    |
| 27  | DA    | 568 | U    |
| 27  | DA    | 571 | A    |
| 27  | DA    | 572 | A    |
| 27  | DA    | 573 | G    |
| 27  | DA    | 575 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 27  | DA    | 583    | G    |
| 27  | DA    | 587    | C    |
| 27  | DA    | 588    | U    |
| 27  | DA    | 594    | U    |
| 27  | DA    | 602    | G    |
| 27  | DA    | 604    | G    |
| 27  | DA    | 607    | U    |
| 27  | DA    | 614(B) | G    |
| 27  | DA    | 614(C) | A    |
| 27  | DA    | 615    | G    |
| 27  | DA    | 620    | G    |
| 27  | DA    | 621    | A    |
| 27  | DA    | 622    | G    |
| 27  | DA    | 623    | G    |
| 27  | DA    | 627    | A    |
| 27  | DA    | 628    | G    |
| 27  | DA    | 629    | G    |
| 27  | DA    | 631    | A    |
| 27  | DA    | 632    | A    |
| 27  | DA    | 634    | C    |
| 27  | DA    | 635    | C    |
| 27  | DA    | 638    | G    |
| 27  | DA    | 645    | C    |
| 27  | DA    | 646    | A    |
| 27  | DA    | 657    | U    |
| 27  | DA    | 668    | G    |
| 27  | DA    | 669    | G    |
| 27  | DA    | 676    | A    |
| 27  | DA    | 686    | G    |
| 27  | DA    | 702    | G    |
| 27  | DA    | 705    | A    |
| 27  | DA    | 707    | G    |
| 27  | DA    | 708    | C    |
| 27  | DA    | 715    | G    |
| 27  | DA    | 720    | C    |
| 27  | DA    | 722    | A    |
| 27  | DA    | 726    | G    |
| 27  | DA    | 727    | A    |
| 27  | DA    | 728    | G    |
| 27  | DA    | 730    | C    |
| 27  | DA    | 740    | U    |
| 27  | DA    | 741    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DA    | 747 | U    |
| 27  | DA    | 748 | G    |
| 27  | DA    | 753 | C    |
| 27  | DA    | 762 | U    |
| 27  | DA    | 763 | G    |
| 27  | DA    | 764 | A    |
| 27  | DA    | 765 | G    |
| 27  | DA    | 776 | G    |
| 27  | DA    | 782 | A    |
| 27  | DA    | 784 | A    |
| 27  | DA    | 785 | G    |
| 27  | DA    | 792 | G    |
| 27  | DA    | 794 | G    |
| 27  | DA    | 795 | C    |
| 27  | DA    | 800 | A    |
| 27  | DA    | 801 | G    |
| 27  | DA    | 805 | G    |
| 27  | DA    | 806 | C    |
| 27  | DA    | 812 | C    |
| 27  | DA    | 817 | C    |
| 27  | DA    | 819 | A    |
| 27  | DA    | 822 | U    |
| 27  | DA    | 827 | U    |
| 27  | DA    | 828 | U    |
| 27  | DA    | 830 | G    |
| 27  | DA    | 831 | G    |
| 27  | DA    | 848 | G    |
| 27  | DA    | 856 | C    |
| 27  | DA    | 857 | C    |
| 27  | DA    | 859 | G    |
| 27  | DA    | 863 | A    |
| 27  | DA    | 865 | C    |
| 27  | DA    | 866 | A    |
| 27  | DA    | 867 | C    |
| 27  | DA    | 872 | A    |
| 27  | DA    | 888 | C    |
| 27  | DA    | 890 | A    |
| 27  | DA    | 896 | A    |
| 27  | DA    | 897 | C    |
| 27  | DA    | 900 | A    |
| 27  | DA    | 904 | C    |
| 27  | DA    | 907 | U    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 27         | DA           | 910        | A           |
| 27         | DA           | 917        | A           |
| 27         | DA           | 926        | A           |
| 27         | DA           | 927        | G           |
| 27         | DA           | 928        | G           |
| 27         | DA           | 932        | G           |
| 27         | DA           | 933        | A           |
| 27         | DA           | 941        | A           |
| 27         | DA           | 945        | A           |
| 27         | DA           | 946        | G           |
| 27         | DA           | 955        | C           |
| 27         | DA           | 957        | A           |
| 27         | DA           | 958        | U           |
| 27         | DA           | 959        | A           |
| 27         | DA           | 960        | A           |
| 27         | DA           | 961        | C           |
| 27         | DA           | 965        | C           |
| 27         | DA           | 966        | G           |
| 27         | DA           | 970        | C           |
| 27         | DA           | 974        | G           |
| 27         | DA           | 975        | C           |
| 27         | DA           | 980        | A           |
| 27         | DA           | 983        | A           |
| 27         | DA           | 986        | C           |
| 27         | DA           | 989        | G           |
| 27         | DA           | 990        | A           |
| 27         | DA           | 991        | C           |
| 27         | DA           | 996        | A           |
| 27         | DA           | 997        | G           |
| 27         | DA           | 999        | U           |
| 27         | DA           | 1000       | A           |
| 27         | DA           | 1004       | C           |
| 27         | DA           | 1005       | C           |
| 27         | DA           | 1008       | C           |
| 27         | DA           | 1009       | A           |
| 27         | DA           | 1010       | A           |
| 27         | DA           | 1011       | G           |
| 27         | DA           | 1012       | U           |
| 27         | DA           | 1013       | C           |
| 27         | DA           | 1015       | G           |
| 27         | DA           | 1020       | A           |
| 27         | DA           | 1021       | A           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | DA    | 1022    | G    |
| 27  | DA    | 1023    | U    |
| 27  | DA    | 1025    | G    |
| 27  | DA    | 1026    | U    |
| 27  | DA    | 1027    | A    |
| 27  | DA    | 1031    | G    |
| 27  | DA    | 1033    | U    |
| 27  | DA    | 1034    | G    |
| 27  | DA    | 1035    | U    |
| 27  | DA    | 1036    | G    |
| 27  | DA    | 1039    | G    |
| 27  | DA    | 1040    | C    |
| 27  | DA    | 1044    | G    |
| 27  | DA    | 1045    | A    |
| 27  | DA    | 1047    | G    |
| 27  | DA    | 1049    | C    |
| 27  | DA    | 1050    | A    |
| 27  | DA    | 1051    | G    |
| 27  | DA    | 1053    | C    |
| 27  | DA    | 1054    | A    |
| 27  | DA    | 1055    | G    |
| 27  | DA    | 1110    | G    |
| 27  | DA    | 1111    | A    |
| 27  | DA    | 1112    | G    |
| 27  | DA    | 1115    | G    |
| 27  | DA    | 1126    | A    |
| 27  | DA    | 1127    | A    |
| 27  | DA    | 1128    | A    |
| 27  | DA    | 1130    | U    |
| 27  | DA    | 1132    | A    |
| 27  | DA    | 1133    | U    |
| 27  | DA    | 1135    | C    |
| 27  | DA    | 1136    | G    |
| 27  | DA    | 1142    | U    |
| 27  | DA    | 1142(A) | A    |
| 27  | DA    | 1143    | A    |
| 27  | DA    | 1144    | G    |
| 27  | DA    | 1155    | A    |
| 27  | DA    | 1157    | G    |
| 27  | DA    | 1158    | C    |
| 27  | DA    | 1159    | U    |
| 27  | DA    | 1171    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | DA    | 1173 | G    |
| 27  | DA    | 1174 | A    |
| 27  | DA    | 1175 | U    |
| 27  | DA    | 1176 | G    |
| 27  | DA    | 1177 | A    |
| 27  | DA    | 1179 | C    |
| 27  | DA    | 1180 | C    |
| 27  | DA    | 1186 | G    |
| 27  | DA    | 1195 | G    |
| 27  | DA    | 1204 | A    |
| 27  | DA    | 1205 | U    |
| 27  | DA    | 1206 | G    |
| 27  | DA    | 1207 | C    |
| 27  | DA    | 1208 | C    |
| 27  | DA    | 1210 | A    |
| 27  | DA    | 1211 | U    |
| 27  | DA    | 1216 | G    |
| 27  | DA    | 1220 | A    |
| 27  | DA    | 1221 | C    |
| 27  | DA    | 1236 | G    |
| 27  | DA    | 1237 | A    |
| 27  | DA    | 1238 | G    |
| 27  | DA    | 1243 | G    |
| 27  | DA    | 1247 | A    |
| 27  | DA    | 1248 | G    |
| 27  | DA    | 1251 | C    |
| 27  | DA    | 1252 | G    |
| 27  | DA    | 1253 | A    |
| 27  | DA    | 1255 | U    |
| 27  | DA    | 1256 | G    |
| 27  | DA    | 1265 | A    |
| 27  | DA    | 1267 | U    |
| 27  | DA    | 1268 | A    |
| 27  | DA    | 1271 | G    |
| 27  | DA    | 1272 | A    |
| 27  | DA    | 1273 | U    |
| 27  | DA    | 1276 | A    |
| 27  | DA    | 1281 | G    |
| 27  | DA    | 1285 | G    |
| 27  | DA    | 1288 | U    |
| 27  | DA    | 1289 | C    |
| 27  | DA    | 1290 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | DA    | 1294 | U    |
| 27  | DA    | 1300 | U    |
| 27  | DA    | 1301 | A    |
| 27  | DA    | 1302 | A    |
| 27  | DA    | 1311 | G    |
| 27  | DA    | 1312 | U    |
| 27  | DA    | 1314 | C    |
| 27  | DA    | 1319 | G    |
| 27  | DA    | 1320 | C    |
| 27  | DA    | 1321 | A    |
| 27  | DA    | 1322 | A    |
| 27  | DA    | 1325 | G    |
| 27  | DA    | 1329 | U    |
| 27  | DA    | 1332 | G    |
| 27  | DA    | 1333 | C    |
| 27  | DA    | 1341 | U    |
| 27  | DA    | 1345 | C    |
| 27  | DA    | 1349 | A    |
| 27  | DA    | 1352 | U    |
| 27  | DA    | 1354 | A    |
| 27  | DA    | 1355 | G    |
| 27  | DA    | 1359 | A    |
| 27  | DA    | 1365 | A    |
| 27  | DA    | 1368 | G    |
| 27  | DA    | 1379 | A    |
| 27  | DA    | 1380 | G    |
| 27  | DA    | 1384 | A    |
| 27  | DA    | 1386 | C    |
| 27  | DA    | 1387 | C    |
| 27  | DA    | 1393 | A    |
| 27  | DA    | 1395 | A    |
| 27  | DA    | 1396 | U    |
| 27  | DA    | 1397 | U    |
| 27  | DA    | 1398 | C    |
| 27  | DA    | 1399 | C    |
| 27  | DA    | 1407 | C    |
| 27  | DA    | 1416 | G    |
| 27  | DA    | 1419 | A    |
| 27  | DA    | 1420 | U    |
| 27  | DA    | 1421 | G    |
| 27  | DA    | 1427 | A    |
| 27  | DA    | 1428 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | DA    | 1437    | C    |
| 27  | DA    | 1445    | A    |
| 27  | DA    | 1445(A) | C    |
| 27  | DA    | 1448    | G    |
| 27  | DA    | 1449    | A    |
| 27  | DA    | 1452    | A    |
| 27  | DA    | 1453    | U    |
| 27  | DA    | 1455    | G    |
| 27  | DA    | 1459    | G    |
| 27  | DA    | 1460    | A    |
| 27  | DA    | 1461    | G    |
| 27  | DA    | 1467    | C    |
| 27  | DA    | 1471    | A    |
| 27  | DA    | 1478    | G    |
| 27  | DA    | 1481    | U    |
| 27  | DA    | 1482    | G    |
| 27  | DA    | 1484    | G    |
| 27  | DA    | 1485    | G    |
| 27  | DA    | 1490    | A    |
| 27  | DA    | 1493    | C    |
| 27  | DA    | 1494    | A    |
| 27  | DA    | 1495    | A    |
| 27  | DA    | 1496    | A    |
| 27  | DA    | 1497    | U    |
| 27  | DA    | 1498    | C    |
| 27  | DA    | 1502    | C    |
| 27  | DA    | 1505    | C    |
| 27  | DA    | 1507    | A    |
| 27  | DA    | 1509    | C    |
| 27  | DA    | 1509(A) | A    |
| 27  | DA    | 1516    | C    |
| 27  | DA    | 1519    | G    |
| 27  | DA    | 1520    | G    |
| 27  | DA    | 1523    | U    |
| 27  | DA    | 1546    | C    |
| 27  | DA    | 1547    | C    |
| 27  | DA    | 1549    | C    |
| 27  | DA    | 1554    | A    |
| 27  | DA    | 1555    | G    |
| 27  | DA    | 1558    | A    |
| 27  | DA    | 1559    | G    |
| 27  | DA    | 1560    | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | DA    | 1566    | A    |
| 27  | DA    | 1569    | A    |
| 27  | DA    | 1575    | C    |
| 27  | DA    | 1578    | U    |
| 27  | DA    | 1579    | A    |
| 27  | DA    | 1580    | A    |
| 27  | DA    | 1581    | G    |
| 27  | DA    | 1584    | C    |
| 27  | DA    | 1586    | A    |
| 27  | DA    | 1588    | C    |
| 27  | DA    | 1591    | G    |
| 27  | DA    | 1602    | U    |
| 27  | DA    | 1603    | A    |
| 27  | DA    | 1604    | C    |
| 27  | DA    | 1607    | C    |
| 27  | DA    | 1608    | A    |
| 27  | DA    | 1609    | A    |
| 27  | DA    | 1610    | A    |
| 27  | DA    | 1611    | C    |
| 27  | DA    | 1615    | C    |
| 27  | DA    | 1616    | A    |
| 27  | DA    | 1617    | C    |
| 27  | DA    | 1618    | A    |
| 27  | DA    | 1622    | G    |
| 27  | DA    | 1625    | C    |
| 27  | DA    | 1631(A) | A    |
| 27  | DA    | 1634    | A    |
| 27  | DA    | 1635    | G    |
| 27  | DA    | 1640    | C    |
| 27  | DA    | 1648    | C    |
| 27  | DA    | 1654    | A    |
| 27  | DA    | 1674    | G    |
| 27  | DA    | 1675    | C    |
| 27  | DA    | 1681    | G    |
| 27  | DA    | 1682    | G    |
| 27  | DA    | 1686    | C    |
| 27  | DA    | 1688    | U    |
| 27  | DA    | 1694    | C    |
| 27  | DA    | 1695    | G    |
| 27  | DA    | 1696    | G    |
| 27  | DA    | 1699    | G    |
| 27  | DA    | 1700    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | DA    | 1701    | A    |
| 27  | DA    | 1702    | G    |
| 27  | DA    | 1703    | G    |
| 27  | DA    | 1718    | G    |
| 27  | DA    | 1721    | G    |
| 27  | DA    | 1722    | A    |
| 27  | DA    | 1739    | U    |
| 27  | DA    | 1740    | G    |
| 27  | DA    | 1741    | A    |
| 27  | DA    | 1742    | G    |
| 27  | DA    | 1744    | C    |
| 27  | DA    | 1745(A) | C    |
| 27  | DA    | 1748    | G    |
| 27  | DA    | 1753    | G    |
| 27  | DA    | 1754    | C    |
| 27  | DA    | 1756    | G    |
| 27  | DA    | 1758    | G    |
| 27  | DA    | 1759    | A    |
| 27  | DA    | 1763    | G    |
| 27  | DA    | 1764    | G    |
| 27  | DA    | 1773    | A    |
| 27  | DA    | 1778    | U    |
| 27  | DA    | 1780    | A    |
| 27  | DA    | 1782    | C    |
| 27  | DA    | 1783    | A    |
| 27  | DA    | 1785    | A    |
| 27  | DA    | 1787    | A    |
| 27  | DA    | 1791    | A    |
| 27  | DA    | 1799    | G    |
| 27  | DA    | 1800    | C    |
| 27  | DA    | 1801    | G    |
| 27  | DA    | 1803    | A    |
| 27  | DA    | 1815    | A    |
| 27  | DA    | 1816    | G    |
| 27  | DA    | 1819    | A    |
| 27  | DA    | 1820    | U    |
| 27  | DA    | 1827    | C    |
| 27  | DA    | 1828    | G    |
| 27  | DA    | 1829    | A    |
| 27  | DA    | 1838    | C    |
| 27  | DA    | 1839    | G    |
| 27  | DA    | 1847    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | DA    | 1848 | A    |
| 27  | DA    | 1858 | G    |
| 27  | DA    | 1865 | G    |
| 27  | DA    | 1877 | A    |
| 27  | DA    | 1878 | G    |
| 27  | DA    | 1882 | C    |
| 27  | DA    | 1885 | A    |
| 27  | DA    | 1888 | G    |
| 27  | DA    | 1889 | A    |
| 27  | DA    | 1894 | C    |
| 27  | DA    | 1900 | A    |
| 27  | DA    | 1901 | A    |
| 27  | DA    | 1906 | G    |
| 27  | DA    | 1908 | C    |
| 27  | DA    | 1912 | A    |
| 27  | DA    | 1913 | A    |
| 27  | DA    | 1926 | U    |
| 27  | DA    | 1929 | G    |
| 27  | DA    | 1930 | G    |
| 27  | DA    | 1937 | A    |
| 27  | DA    | 1938 | A    |
| 27  | DA    | 1943 | U    |
| 27  | DA    | 1944 | U    |
| 27  | DA    | 1945 | G    |
| 27  | DA    | 1954 | G    |
| 27  | DA    | 1955 | U    |
| 27  | DA    | 1956 | U    |
| 27  | DA    | 1957 | C    |
| 27  | DA    | 1962 | C    |
| 27  | DA    | 1963 | U    |
| 27  | DA    | 1965 | C    |
| 27  | DA    | 1966 | A    |
| 27  | DA    | 1967 | C    |
| 27  | DA    | 1969 | A    |
| 27  | DA    | 1970 | A    |
| 27  | DA    | 1971 | A    |
| 27  | DA    | 1972 | A    |
| 27  | DA    | 1982 | C    |
| 27  | DA    | 1987 | G    |
| 27  | DA    | 1993 | U    |
| 27  | DA    | 1996 | C    |
| 27  | DA    | 1997 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | DA    | 2004 | G    |
| 27  | DA    | 2019 | A    |
| 27  | DA    | 2021 | C    |
| 27  | DA    | 2022 | U    |
| 27  | DA    | 2023 | G    |
| 27  | DA    | 2024 | G    |
| 27  | DA    | 2025 | C    |
| 27  | DA    | 2030 | A    |
| 27  | DA    | 2031 | A    |
| 27  | DA    | 2032 | G    |
| 27  | DA    | 2033 | A    |
| 27  | DA    | 2034 | U    |
| 27  | DA    | 2035 | G    |
| 27  | DA    | 2036 | C    |
| 27  | DA    | 2037 | G    |
| 27  | DA    | 2039 | C    |
| 27  | DA    | 2043 | C    |
| 27  | DA    | 2052 | G    |
| 27  | DA    | 2055 | C    |
| 27  | DA    | 2056 | G    |
| 27  | DA    | 2060 | A    |
| 27  | DA    | 2061 | G    |
| 27  | DA    | 2062 | A    |
| 27  | DA    | 2063 | C    |
| 27  | DA    | 2066 | C    |
| 27  | DA    | 2067 | G    |
| 27  | DA    | 2068 | U    |
| 27  | DA    | 2069 | G    |
| 27  | DA    | 2090 | G    |
| 27  | DA    | 2092 | U    |
| 27  | DA    | 2093 | G    |
| 27  | DA    | 2098 | U    |
| 27  | DA    | 2099 | U    |
| 27  | DA    | 2103 | C    |
| 27  | DA    | 2104 | G    |
| 27  | DA    | 2111 | C    |
| 27  | DA    | 2113 | U    |
| 27  | DA    | 2114 | A    |
| 27  | DA    | 2116 | G    |
| 27  | DA    | 2117 | A    |
| 27  | DA    | 2118 | U    |
| 27  | DA    | 2119 | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 27         | DA           | 2120       | G           |
| 27         | DA           | 2121       | G           |
| 27         | DA           | 2126       | A           |
| 27         | DA           | 2127       | G           |
| 27         | DA           | 2128       | C           |
| 27         | DA           | 2131       | G           |
| 27         | DA           | 2133       | G           |
| 27         | DA           | 2136       | C           |
| 27         | DA           | 2144       | U           |
| 27         | DA           | 2146       | C           |
| 27         | DA           | 2147       | G           |
| 27         | DA           | 2148       | G           |
| 27         | DA           | 2157       | G           |
| 27         | DA           | 2159       | G           |
| 27         | DA           | 2160       | G           |
| 27         | DA           | 2172       | U           |
| 27         | DA           | 2173       | A           |
| 27         | DA           | 2174       | C           |
| 27         | DA           | 2175       | C           |
| 27         | DA           | 2176       | A           |
| 27         | DA           | 2179       | C           |
| 27         | DA           | 2187       | G           |
| 27         | DA           | 2189       | U           |
| 27         | DA           | 2190       | G           |
| 27         | DA           | 2192       | G           |
| 27         | DA           | 2193       | G           |
| 27         | DA           | 2196       | C           |
| 27         | DA           | 2197       | U           |
| 27         | DA           | 2198       | A           |
| 27         | DA           | 2199       | A           |
| 27         | DA           | 2200       | C           |
| 27         | DA           | 2207       | G           |
| 27         | DA           | 2208       | A           |
| 27         | DA           | 2218       | U           |
| 27         | DA           | 2219       | G           |
| 27         | DA           | 2222       | G           |
| 27         | DA           | 2225       | A           |
| 27         | DA           | 2226       | C           |
| 27         | DA           | 2227       | A           |
| 27         | DA           | 2234       | G           |
| 27         | DA           | 2238       | G           |
| 27         | DA           | 2239       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | DA    | 2246 | G    |
| 27  | DA    | 2250 | G    |
| 27  | DA    | 2251 | G    |
| 27  | DA    | 2255 | G    |
| 27  | DA    | 2259 | G    |
| 27  | DA    | 2266 | A    |
| 27  | DA    | 2267 | A    |
| 27  | DA    | 2268 | A    |
| 27  | DA    | 2275 | C    |
| 27  | DA    | 2276 | G    |
| 27  | DA    | 2277 | G    |
| 27  | DA    | 2283 | C    |
| 27  | DA    | 2286 | A    |
| 27  | DA    | 2287 | A    |
| 27  | DA    | 2288 | A    |
| 27  | DA    | 2289 | G    |
| 27  | DA    | 2290 | G    |
| 27  | DA    | 2296 | U    |
| 27  | DA    | 2297 | C    |
| 27  | DA    | 2304 | G    |
| 27  | DA    | 2305 | A    |
| 27  | DA    | 2307 | G    |
| 27  | DA    | 2308 | G    |
| 27  | DA    | 2309 | A    |
| 27  | DA    | 2310 | A    |
| 27  | DA    | 2311 | A    |
| 27  | DA    | 2312 | U    |
| 27  | DA    | 2313 | C    |
| 27  | DA    | 2316 | C    |
| 27  | DA    | 2319 | G    |
| 27  | DA    | 2320 | A    |
| 27  | DA    | 2321 | G    |
| 27  | DA    | 2322 | A    |
| 27  | DA    | 2325 | G    |
| 27  | DA    | 2327 | A    |
| 27  | DA    | 2330 | G    |
| 27  | DA    | 2334 | G    |
| 27  | DA    | 2335 | A    |
| 27  | DA    | 2336 | A    |
| 27  | DA    | 2338 | G    |
| 27  | DA    | 2345 | G    |
| 27  | DA    | 2346 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | DA    | 2347 | C    |
| 27  | DA    | 2349 | G    |
| 27  | DA    | 2355 | C    |
| 27  | DA    | 2383 | G    |
| 27  | DA    | 2384 | G    |
| 27  | DA    | 2385 | C    |
| 27  | DA    | 2387 | U    |
| 27  | DA    | 2392 | A    |
| 27  | DA    | 2395 | C    |
| 27  | DA    | 2398 | U    |
| 27  | DA    | 2399 | G    |
| 27  | DA    | 2400 | G    |
| 27  | DA    | 2402 | C    |
| 27  | DA    | 2403 | C    |
| 27  | DA    | 2406 | U    |
| 27  | DA    | 2422 | A    |
| 27  | DA    | 2423 | U    |
| 27  | DA    | 2424 | C    |
| 27  | DA    | 2425 | A    |
| 27  | DA    | 2427 | C    |
| 27  | DA    | 2428 | G    |
| 27  | DA    | 2429 | G    |
| 27  | DA    | 2430 | A    |
| 27  | DA    | 2431 | U    |
| 27  | DA    | 2434 | A    |
| 27  | DA    | 2439 | A    |
| 27  | DA    | 2440 | C    |
| 27  | DA    | 2441 | C    |
| 27  | DA    | 2447 | G    |
| 27  | DA    | 2448 | A    |
| 27  | DA    | 2452 | C    |
| 27  | DA    | 2458 | G    |
| 27  | DA    | 2459 | A    |
| 27  | DA    | 2460 | U    |
| 27  | DA    | 2469 | A    |
| 27  | DA    | 2470 | G    |
| 27  | DA    | 2476 | A    |
| 27  | DA    | 2477 | C    |
| 27  | DA    | 2482 | G    |
| 27  | DA    | 2483 | C    |
| 27  | DA    | 2484 | G    |
| 27  | DA    | 2490 | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 27         | DA           | 2491       | U           |
| 27         | DA           | 2495       | G           |
| 27         | DA           | 2498       | C           |
| 27         | DA           | 2499       | C           |
| 27         | DA           | 2502       | G           |
| 27         | DA           | 2505       | G           |
| 27         | DA           | 2518       | A           |
| 27         | DA           | 2520       | C           |
| 27         | DA           | 2522       | U           |
| 27         | DA           | 2523       | G           |
| 27         | DA           | 2527       | C           |
| 27         | DA           | 2529       | G           |
| 27         | DA           | 2534       | A           |
| 27         | DA           | 2538       | C           |
| 27         | DA           | 2543       | G           |
| 27         | DA           | 2546       | U           |
| 27         | DA           | 2547       | U           |
| 27         | DA           | 2553       | G           |
| 27         | DA           | 2554       | U           |
| 27         | DA           | 2566       | A           |
| 27         | DA           | 2567       | G           |
| 27         | DA           | 2569       | G           |
| 27         | DA           | 2572       | A           |
| 27         | DA           | 2573       | C           |
| 27         | DA           | 2577       | A           |
| 27         | DA           | 2579       | C           |
| 27         | DA           | 2580       | U           |
| 27         | DA           | 2581       | G           |
| 27         | DA           | 2585       | U           |
| 27         | DA           | 2586       | C           |
| 27         | DA           | 2587       | A           |
| 27         | DA           | 2598       | A           |
| 27         | DA           | 2599       | G           |
| 27         | DA           | 2602       | A           |
| 27         | DA           | 2603       | G           |
| 27         | DA           | 2608       | G           |
| 27         | DA           | 2609       | U           |
| 27         | DA           | 2610       | C           |
| 27         | DA           | 2611       | U           |
| 27         | DA           | 2612       | C           |
| 27         | DA           | 2613       | U           |
| 27         | DA           | 2629       | A           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | DA    | 2630    | G    |
| 27  | DA    | 2632    | A    |
| 27  | DA    | 2636    | U    |
| 27  | DA    | 2639    | A    |
| 27  | DA    | 2645    | G    |
| 27  | DA    | 2646    | C    |
| 27  | DA    | 2654    | A    |
| 27  | DA    | 2655    | G    |
| 27  | DA    | 2656    | U    |
| 27  | DA    | 2657    | A    |
| 27  | DA    | 2673    | G    |
| 27  | DA    | 2682    | U    |
| 27  | DA    | 2683    | C    |
| 27  | DA    | 2686    | G    |
| 27  | DA    | 2690    | C    |
| 27  | DA    | 2691    | C    |
| 27  | DA    | 2702    | U    |
| 27  | DA    | 2703    | C    |
| 27  | DA    | 2707    | G    |
| 27  | DA    | 2712    | U    |
| 27  | DA    | 2712(A) | A    |
| 27  | DA    | 2713    | A    |
| 27  | DA    | 2714    | G    |
| 27  | DA    | 2715    | C    |
| 27  | DA    | 2726    | U    |
| 27  | DA    | 2727    | G    |
| 27  | DA    | 2730    | C    |
| 27  | DA    | 2732    | G    |
| 27  | DA    | 2733    | A    |
| 27  | DA    | 2739    | U    |
| 27  | DA    | 2748    | A    |
| 27  | DA    | 2750    | A    |
| 27  | DA    | 2751    | G    |
| 27  | DA    | 2752    | C    |
| 27  | DA    | 2754    | U    |
| 27  | DA    | 2756    | U    |
| 27  | DA    | 2757    | A    |
| 27  | DA    | 2758    | A    |
| 27  | DA    | 2759    | G    |
| 27  | DA    | 2762    | G    |
| 27  | DA    | 2763    | G    |
| 27  | DA    | 2764    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 27  | DA    | 2765    | A    |
| 27  | DA    | 2777    | G    |
| 27  | DA    | 2778    | A    |
| 27  | DA    | 2780    | G    |
| 27  | DA    | 2789    | C    |
| 27  | DA    | 2791    | C    |
| 27  | DA    | 2792    | G    |
| 27  | DA    | 2794    | C    |
| 27  | DA    | 2795    | G    |
| 27  | DA    | 2796    | U    |
| 27  | DA    | 2799    | C    |
| 27  | DA    | 2801(A) | A    |
| 27  | DA    | 2802    | G    |
| 27  | DA    | 2803    | C    |
| 27  | DA    | 2804    | C    |
| 27  | DA    | 2805    | G    |
| 27  | DA    | 2807    | G    |
| 27  | DA    | 2808    | U    |
| 27  | DA    | 2818    | G    |
| 27  | DA    | 2820    | A    |
| 27  | DA    | 2821    | A    |
| 27  | DA    | 2827    | C    |
| 27  | DA    | 2833    | G    |
| 27  | DA    | 2834    | G    |
| 27  | DA    | 2835    | A    |
| 27  | DA    | 2849    | U    |
| 27  | DA    | 2861    | G    |
| 27  | DA    | 2866    | U    |
| 27  | DA    | 2867    | G    |
| 27  | DA    | 2872    | G    |
| 27  | DA    | 2874    | C    |
| 27  | DA    | 2875    | C    |
| 27  | DA    | 2879    | C    |
| 27  | DA    | 2880    | C    |
| 27  | DA    | 2883    | A    |
| 27  | DA    | 2889    | C    |
| 27  | DA    | 2893    | G    |
| 27  | DA    | 2894    | G    |
| 27  | DA    | 2895    | U    |
| 27  | DA    | 2896    | C    |
| 28  | DB    | 2       | C    |
| 28  | DB    | 8       | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DB    | 12  | C    |
| 28  | DB    | 13  | A    |
| 28  | DB    | 15  | A    |
| 28  | DB    | 25  | A    |
| 28  | DB    | 26  | A    |
| 28  | DB    | 27  | C    |
| 28  | DB    | 28  | C    |
| 28  | DB    | 34  | U    |
| 28  | DB    | 35  | U    |
| 28  | DB    | 36  | C    |
| 28  | DB    | 40  | U    |
| 28  | DB    | 42  | C    |
| 28  | DB    | 45  | A    |
| 28  | DB    | 46  | A    |
| 28  | DB    | 52  | A    |
| 28  | DB    | 53  | A    |
| 28  | DB    | 60  | C    |
| 28  | DB    | 63  | G    |
| 28  | DB    | 67  | G    |
| 28  | DB    | 73  | A    |
| 28  | DB    | 77  | U    |
| 28  | DB    | 88  | C    |
| 28  | DB    | 90  | A    |
| 28  | DB    | 91  | C    |
| 28  | DB    | 110 | G    |
| 28  | DB    | 113 | G    |

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | KBE  | AZ    | 1   | 26   | 8,8,9        | 0.56 | 0        | 7,8,10      | 1.28 | 1 (14%)  |
| 26  | DPP  | AZ    | 2   | 26   | 4,5,6        | 0.34 | 0        | 1,5,7       | 0.64 | 0        |
| 26  | UAL  | AZ    | 5   | 26   | 8,8,9        | 2.34 | 3 (37%)  | 4,9,11      | 1.31 | 1 (25%)  |
| 26  | 5OH  | AZ    | 6   | 26   | 8,12,13      | 1.06 | 1 (12%)  | 5,16,18     | 0.83 | 0        |
| 26  | KBE  | CZ    | 1   | 26   | 8,8,9        | 0.60 | 0        | 7,8,10      | 0.74 | 0        |
| 26  | DPP  | CZ    | 2   | 26   | 4,5,6        | 1.16 | 0        | 1,5,7       | 1.41 | 0        |
| 26  | UAL  | CZ    | 5   | 26   | 8,8,9        | 2.93 | 3 (37%)  | 4,9,11      | 3.86 | 3 (75%)  |
| 26  | 5OH  | CZ    | 6   | 26   | 8,12,13      | 0.65 | 0        | 5,16,18     | 0.99 | 1 (20%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 26  | KBE  | AZ    | 1   | 26   | -       | 0/7/7/8   | 0/0/0/0 |
| 26  | DPP  | AZ    | 2   | 26   | -       | 0/2/4/6   | 0/0/0/0 |
| 26  | UAL  | AZ    | 5   | 26   | -       | 0/3/7/9   | 0/0/0/0 |
| 26  | 5OH  | AZ    | 6   | 26   | -       | 0/2/18/20 | 0/1/1/1 |
| 26  | KBE  | CZ    | 1   | 26   | -       | 0/7/7/8   | 0/0/0/0 |
| 26  | DPP  | CZ    | 2   | 26   | -       | 0/2/4/6   | 0/0/0/0 |
| 26  | UAL  | CZ    | 5   | 26   | -       | 0/3/7/9   | 0/0/0/0 |
| 26  | 5OH  | CZ    | 6   | 26   | -       | 0/2/18/20 | 0/1/1/1 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 26  | CZ    | 5   | UAL  | C1-N1 | -6.17 | 1.29        | 1.40     |
| 26  | AZ    | 5   | UAL  | C1-N1 | -2.86 | 1.35        | 1.40     |
| 26  | AZ    | 5   | UAL  | CB-CA | 2.20  | 1.41        | 1.35     |
| 26  | AZ    | 6   | 5OH  | CA-C  | 2.69  | 1.53        | 1.50     |
| 26  | CZ    | 5   | UAL  | CB-CA | 3.57  | 1.44        | 1.35     |
| 26  | CZ    | 5   | UAL  | C-CA  | 3.62  | 1.51        | 1.45     |
| 26  | AZ    | 5   | UAL  | C-CA  | 5.01  | 1.53        | 1.45     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 26  | CZ    | 5   | UAL  | O2-C1-N2 | -6.52 | 111.92      | 123.12   |
| 26  | AZ    | 5   | UAL  | O-C-CA   | -2.37 | 122.45      | 125.47   |
| 26  | CZ    | 6   | 5OH  | O-C-CA   | -2.14 | 120.15      | 125.15   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 26  | CZ    | 5   | UAL  | N2-C1-N1 | 2.58 | 121.55      | 115.75   |
| 26  | CZ    | 5   | UAL  | O2-C1-N1 | 2.70 | 126.51      | 120.04   |
| 26  | AZ    | 1   | KBE  | CB-CA-C  | 2.71 | 116.35      | 112.25   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 26  | AZ    | 1   | KBE  | 3       | 0            |
| 26  | AZ    | 5   | UAL  | 3       | 0            |
| 26  | AZ    | 6   | 5OH  | 3       | 0            |
| 26  | CZ    | 1   | KBE  | 1       | 0            |
| 26  | CZ    | 5   | UAL  | 4       | 0            |
| 26  | CZ    | 6   | 5OH  | 11      | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 973 ligands modelled in this entry, 973 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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    | 1495/1509 (99%) | -0.10  | 30 (2%) 65 36 | 48, 83, 149, 196      | 0     |
| 1   | CA    | 1495/1509 (99%) | -0.04  | 32 (2%) 64 34 | 59, 91, 155, 196      | 0     |
| 2   | AB    | 235/256 (91%)   | 0.18   | 15 (6%) 20 7  | 80, 114, 144, 161     | 0     |
| 2   | CB    | 235/256 (91%)   | 0.07   | 13 (5%) 26 10 | 81, 118, 152, 171     | 0     |
| 3   | AC    | 207/239 (86%)   | -0.09  | 4 (1%) 67 37  | 76, 101, 140, 153     | 0     |
| 3   | CC    | 207/239 (86%)   | 0.02   | 9 (4%) 36 15  | 89, 109, 136, 147     | 0     |
| 4   | AD    | 208/209 (99%)   | -0.08  | 9 (4%) 36 15  | 65, 84, 101, 114      | 0     |
| 4   | CD    | 208/209 (99%)   | -0.26  | 3 (1%) 75 49  | 55, 77, 98, 107       | 0     |
| 5   | AE    | 151/162 (93%)   | -0.16  | 2 (1%) 77 51  | 59, 81, 107, 122      | 0     |
| 5   | CE    | 151/162 (93%)   | -0.03  | 0 100 100     | 72, 88, 109, 145      | 0     |
| 6   | AF    | 101/101 (100%)  | -0.30  | 0 100 100     | 63, 84, 93, 110       | 0     |
| 6   | CF    | 101/101 (100%)  | -0.24  | 0 100 100     | 76, 88, 101, 134      | 0     |
| 7   | AG    | 155/156 (99%)   | -0.06  | 9 (5%) 24 9   | 74, 94, 129, 151      | 0     |
| 7   | CG    | 155/156 (99%)   | -0.11  | 6 (3%) 40 16  | 84, 103, 128, 140     | 0     |
| 8   | AH    | 138/138 (100%)  | -0.33  | 0 100 100     | 69, 84, 96, 107       | 0     |
| 8   | CH    | 138/138 (100%)  | -0.18  | 2 (1%) 75 49  | 74, 91, 102, 117      | 0     |
| 9   | AI    | 127/128 (99%)   | 0.34   | 9 (7%) 17 6   | 76, 115, 136, 144     | 0     |
| 9   | CI    | 127/128 (99%)   | 0.20   | 9 (7%) 17 6   | 89, 121, 139, 143     | 0     |
| 10  | AJ    | 99/105 (94%)    | 0.82   | 14 (14%) 3 1  | 80, 127, 152, 164     | 0     |
| 10  | CJ    | 99/105 (94%)    | 0.78   | 11 (11%) 6 2  | 88, 125, 148, 154     | 0     |
| 11  | AK    | 119/129 (92%)   | 0.30   | 12 (10%) 8 3  | 55, 79, 107, 127      | 0     |
| 11  | CK    | 119/129 (92%)   | 0.14   | 10 (8%) 12 4  | 69, 88, 108, 124      | 0     |
| 12  | AL    | 125/132 (94%)   | -0.15  | 0 100 100     | 55, 69, 91, 126       | 0     |
| 12  | CL    | 125/132 (94%)   | 0.17   | 7 (5%) 25 10  | 66, 82, 98, 129       | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-----|-----|-----------------------|-------|
| 13  | AM    | 120/126 (95%)   | -0.26  | 4 (3%)   | 47  | 21  | 58, 86, 98, 107       | 0     |
| 13  | CM    | 119/126 (94%)   | -0.15  | 4 (3%)   | 46  | 20  | 80, 108, 125, 136     | 0     |
| 14  | AN    | 60/61 (98%)     | -0.01  | 1 (1%)   | 70  | 42  | 76, 92, 110, 122      | 0     |
| 14  | CN    | 60/61 (98%)     | 0.30   | 2 (3%)   | 47  | 21  | 90, 105, 120, 123     | 0     |
| 15  | AO    | 88/89 (98%)     | -0.05  | 4 (4%)   | 34  | 13  | 64, 76, 99, 114       | 0     |
| 15  | CO    | 88/89 (98%)     | 0.16   | 2 (2%)   | 61  | 31  | 71, 84, 106, 117      | 0     |
| 16  | AP    | 84/88 (95%)     | 0.01   | 5 (5%)   | 23  | 9   | 68, 86, 108, 124      | 0     |
| 16  | CP    | 84/88 (95%)     | 0.12   | 1 (1%)   | 79  | 53  | 71, 81, 105, 136      | 0     |
| 17  | AQ    | 100/105 (95%)   | 0.16   | 2 (2%)   | 65  | 36  | 62, 79, 95, 99        | 0     |
| 17  | CQ    | 100/105 (95%)   | -0.23  | 0        | 100 | 100 | 64, 85, 100, 103      | 0     |
| 18  | AR    | 70/88 (79%)     | -0.12  | 2 (2%)   | 52  | 24  | 67, 83, 106, 134      | 0     |
| 18  | CR    | 70/88 (79%)     | -0.08  | 0        | 100 | 100 | 73, 86, 107, 134      | 0     |
| 19  | AS    | 79/93 (84%)     | 0.65   | 10 (12%) | 4   | 2   | 87, 105, 127, 134     | 0     |
| 19  | CS    | 79/93 (84%)     | 0.70   | 11 (13%) | 3   | 1   | 101, 122, 143, 154    | 0     |
| 20  | AT    | 99/106 (93%)    | 0.06   | 7 (7%)   | 17  | 6   | 71, 89, 118, 130      | 0     |
| 20  | CT    | 99/106 (93%)    | 0.04   | 7 (7%)   | 17  | 6   | 74, 90, 114, 125      | 0     |
| 21  | AU    | 25/27 (92%)     | 2.00   | 12 (48%) | 0   | 0   | 86, 92, 100, 118      | 0     |
| 21  | CU    | 25/27 (92%)     | 2.33   | 12 (48%) | 0   | 0   | 89, 104, 117, 119     | 0     |
| 22  | AV    | 10/30 (33%)     | 0.45   | 1 (10%)  | 8   | 3   | 63, 73, 124, 133      | 0     |
| 22  | CV    | 10/30 (33%)     | -0.03  | 0        | 100 | 100 | 68, 85, 125, 130      | 0     |
| 23  | AW    | 75/75 (100%)    | 0.73   | 15 (20%) | 1   | 1   | 46, 119, 161, 185     | 0     |
| 23  | CW    | 75/75 (100%)    | 0.50   | 10 (13%) | 4   | 1   | 79, 141, 174, 184     | 0     |
| 24  | AX    | 77/77 (100%)    | 0.06   | 4 (5%)   | 28  | 11  | 48, 89, 121, 130      | 0     |
| 24  | CX    | 77/77 (100%)    | 0.07   | 3 (3%)   | 40  | 16  | 69, 98, 125, 132      | 0     |
| 25  | AY    | 75/75 (100%)    | 1.25   | 25 (33%) | 0   | 0   | 51, 157, 193, 194     | 0     |
| 25  | CY    | 75/75 (100%)    | 1.32   | 23 (30%) | 0   | 0   | 67, 167, 194, 194     | 0     |
| 26  | AZ    | 2/6 (33%)       | 0.41   | 0        | 100 | 100 | 85, 85, 85, 88        | 0     |
| 26  | CZ    | 2/6 (33%)       | 0.75   | 0        | 100 | 100 | 99, 99, 99, 100       | 0     |
| 27  | BA    | 2800/2915 (96%) | -0.12  | 49 (1%)  | 69  | 40  | 30, 56, 157, 198      | 0     |
| 27  | DA    | 2800/2915 (96%) | -0.02  | 72 (2%)  | 56  | 27  | 49, 77, 168, 197      | 0     |
| 28  | BB    | 118/122 (96%)   | -0.22  | 2 (1%)   | 70  | 42  | 47, 76, 119, 164      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28  | DB    | 118/122 (96%)  | -0.00  | 4 (3%) 46 20 | 80, 104, 136, 162     | 0     |
| 29  | BC    | 191/229 (83%)  | 1.64   | 73 (38%) 0 0 | 130, 167, 187, 195    | 0     |
| 29  | DC    | 191/229 (83%)  | 2.08   | 74 (38%) 0 0 | 122, 173, 188, 191    | 0     |
| 30  | BD    | 272/276 (98%)  | -0.39  | 2 (0%) 87 67 | 32, 52, 68, 79        | 0     |
| 30  | DD    | 272/276 (98%)  | -0.33  | 0 100 100    | 46, 61, 78, 92        | 0     |
| 31  | BE    | 205/206 (99%)  | -0.24  | 2 (0%) 82 58 | 33, 58, 93, 104       | 0     |
| 31  | DE    | 205/206 (99%)  | 0.01   | 5 (2%) 59 30 | 57, 84, 112, 121      | 0     |
| 32  | BF    | 208/210 (99%)  | -0.34  | 2 (0%) 82 58 | 29, 60, 125, 149      | 0     |
| 32  | DF    | 208/210 (99%)  | -0.03  | 6 (2%) 52 24 | 54, 86, 132, 152      | 0     |
| 33  | BG    | 181/182 (99%)  | -0.02  | 9 (4%) 30 12 | 64, 83, 116, 146      | 0     |
| 33  | DG    | 181/182 (99%)  | 0.34   | 15 (8%) 12 4 | 79, 106, 132, 153     | 0     |
| 34  | BH    | 164/180 (91%)  | 0.05   | 6 (3%) 42 18 | 68, 97, 124, 142      | 0     |
| 34  | DH    | 160/180 (88%)  | 0.87   | 25 (15%) 2 1 | 110, 139, 159, 163    | 0     |
| 35  | BI    | 146/148 (98%)  | -0.22  | 0 100 100    | 62, 119, 140, 144     | 0     |
| 35  | DI    | 146/148 (98%)  | -0.03  | 3 (2%) 64 34 | 67, 105, 128, 136     | 0     |
| 36  | BN    | 139/140 (99%)  | -0.44  | 0 100 100    | 42, 57, 86, 104       | 0     |
| 36  | DN    | 139/140 (99%)  | -0.26  | 2 (1%) 75 49 | 65, 91, 115, 124      | 0     |
| 37  | BO    | 122/122 (100%) | -0.54  | 1 (0%) 86 64 | 38, 57, 75, 88        | 0     |
| 37  | DO    | 122/122 (100%) | -0.37  | 0 100 100    | 60, 77, 93, 100       | 0     |
| 38  | BP    | 146/150 (97%)  | 0.13   | 5 (3%) 46 20 | 37, 69, 102, 156      | 0     |
| 38  | DP    | 146/150 (97%)  | 0.28   | 4 (2%) 55 26 | 61, 93, 122, 148      | 0     |
| 39  | BQ    | 141/141 (100%) | -0.18  | 2 (1%) 75 49 | 42, 60, 92, 118       | 0     |
| 39  | DQ    | 139/141 (98%)  | -0.18  | 1 (0%) 87 67 | 68, 90, 120, 134      | 0     |
| 40  | BR    | 117/118 (99%)  | -0.36  | 0 100 100    | 35, 52, 69, 82        | 0     |
| 40  | DR    | 117/118 (99%)  | -0.12  | 0 100 100    | 58, 71, 83, 96        | 0     |
| 41  | BS    | 99/112 (88%)   | -0.19  | 0 100 100    | 48, 76, 94, 105       | 0     |
| 41  | DS    | 101/112 (90%)  | 0.31   | 10 (9%) 8 3  | 69, 100, 117, 122     | 0     |
| 42  | BT    | 138/146 (94%)  | -0.13  | 7 (5%) 29 12 | 51, 70, 126, 152      | 0     |
| 42  | DT    | 138/146 (94%)  | 0.13   | 15 (10%) 6 2 | 61, 90, 149, 175      | 0     |
| 43  | BU    | 117/118 (99%)  | -0.22  | 2 (1%) 70 42 | 37, 49, 73, 95        | 0     |
| 43  | DU    | 117/118 (99%)  | 0.32   | 14 (11%) 5 2 | 60, 91, 111, 124      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | BV    | 101/101 (100%)    | -0.46  | 1 (0%) 82 58   | 35, 65, 90, 116       | 0     |
| 44  | DV    | 101/101 (100%)    | 0.29   | 9 (8%) 10 4    | 59, 106, 121, 129     | 0     |
| 45  | BW    | 113/113 (100%)    | -0.30  | 2 (1%) 69 40   | 32, 46, 76, 136       | 0     |
| 45  | DW    | 113/113 (100%)    | -0.36  | 1 (0%) 84 61   | 43, 64, 95, 130       | 0     |
| 46  | BX    | 93/96 (96%)       | -0.32  | 1 (1%) 80 55   | 43, 53, 70, 91        | 0     |
| 46  | DX    | 93/96 (96%)       | -0.28  | 0 100 100      | 56, 71, 89, 95        | 0     |
| 47  | BY    | 101/110 (91%)     | -0.05  | 3 (2%) 51 23   | 58, 78, 145, 163      | 0     |
| 47  | DY    | 101/110 (91%)     | 0.26   | 10 (9%) 8 3    | 73, 94, 149, 156      | 0     |
| 48  | BZ    | 177/206 (85%)     | 0.57   | 24 (13%) 3 1   | 65, 107, 169, 177     | 0     |
| 48  | DZ    | 177/206 (85%)     | 1.28   | 40 (22%) 1 0   | 104, 130, 177, 191    | 0     |
| 49  | B0    | 84/85 (98%)       | -0.16  | 4 (4%) 31 12   | 43, 56, 83, 103       | 0     |
| 49  | D0    | 84/85 (98%)       | 0.48   | 10 (11%) 5 2   | 71, 83, 100, 118      | 0     |
| 50  | B1    | 94/98 (95%)       | -0.21  | 2 (2%) 64 34   | 44, 61, 92, 109       | 0     |
| 50  | D1    | 94/98 (95%)       | 0.06   | 2 (2%) 64 34   | 54, 70, 94, 110       | 0     |
| 51  | B2    | 71/72 (98%)       | -0.37  | 3 (4%) 37 15   | 46, 66, 86, 117       | 0     |
| 51  | D2    | 71/72 (98%)       | -0.30  | 0 100 100      | 65, 86, 103, 107      | 0     |
| 52  | B3    | 60/60 (100%)      | -0.25  | 2 (3%) 47 21   | 43, 58, 85, 110       | 0     |
| 52  | D3    | 60/60 (100%)      | 0.15   | 2 (3%) 47 21   | 75, 90, 112, 116      | 0     |
| 53  | B4    | 31/71 (43%)       | -0.43  | 0 100 100      | 92, 107, 120, 126     | 0     |
| 53  | D4    | 31/71 (43%)       | -0.14  | 0 100 100      | 108, 119, 128, 135    | 0     |
| 54  | B5    | 59/60 (98%)       | -0.23  | 3 (5%) 29 12   | 33, 51, 115, 135      | 0     |
| 54  | D5    | 59/60 (98%)       | -0.01  | 4 (6%) 18 7    | 60, 71, 143, 177      | 0     |
| 55  | B6    | 51/54 (94%)       | 0.17   | 3 (5%) 23 9    | 59, 83, 106, 112      | 0     |
| 55  | D6    | 46/54 (85%)       | 0.80   | 9 (19%) 1 1    | 56, 103, 116, 117     | 0     |
| 56  | B7    | 49/49 (100%)      | -0.17  | 0 100 100      | 28, 44, 84, 115       | 0     |
| 56  | D7    | 49/49 (100%)      | 0.49   | 4 (8%) 12 5    | 46, 59, 90, 101       | 0     |
| 57  | B8    | 64/65 (98%)       | -0.19  | 1 (1%) 72 44   | 40, 56, 73, 97        | 0     |
| 57  | D8    | 64/65 (98%)       | 0.11   | 2 (3%) 49 22   | 60, 74, 87, 118       | 0     |
| 58  | B9    | 36/37 (97%)       | 0.32   | 0 100 100      | 46, 63, 80, 93        | 0     |
| 58  | D9    | 36/37 (97%)       | 1.08   | 10 (27%) 1 0   | 88, 122, 133, 137     | 0     |
| All | All   | 21214/22204 (95%) | 0.02   | 937 (4%) 35 14 | 28, 83, 154, 198      | 0     |

All (937) RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 27  | BA    | 2802    | G    | 15.6 |
| 48  | DZ    | 111     | ARG  | 15.5 |
| 48  | DZ    | 175     | PRO  | 14.5 |
| 27  | DA    | 2802    | G    | 13.1 |
| 29  | DC    | 165     | ASN  | 13.0 |
| 29  | DC    | 133     | PRO  | 12.6 |
| 29  | DC    | 139     | ASN  | 12.4 |
| 7   | AG    | 84      | ASN  | 11.3 |
| 29  | DC    | 149     | ILE  | 11.1 |
| 29  | DC    | 178     | ALA  | 11.1 |
| 33  | DG    | 2       | PRO  | 11.1 |
| 29  | DC    | 179     | SER  | 11.1 |
| 29  | DC    | 150     | GLY  | 10.5 |
| 48  | DZ    | 112     | ALA  | 10.4 |
| 39  | BQ    | 140     | ALA  | 9.6  |
| 27  | BA    | 2801    | A    | 9.2  |
| 29  | BC    | 120     | MET  | 9.0  |
| 47  | BY    | 51      | VAL  | 8.8  |
| 29  | BC    | 179     | SER  | 8.7  |
| 34  | DH    | 171     | LEU  | 8.5  |
| 29  | DC    | 41      | VAL  | 8.5  |
| 48  | DZ    | 106     | THR  | 8.5  |
| 27  | DA    | 2795    | G    | 8.4  |
| 27  | BA    | 2795    | G    | 8.3  |
| 29  | DC    | 176     | GLY  | 8.3  |
| 29  | BC    | 178     | ALA  | 8.2  |
| 25  | AY    | 59      | U    | 8.0  |
| 29  | DC    | 91      | ALA  | 7.8  |
| 34  | BH    | 171     | LEU  | 7.8  |
| 27  | DA    | 2799    | C    | 7.7  |
| 1   | AA    | 1027    | C    | 7.6  |
| 10  | CJ    | 86      | MET  | 7.6  |
| 27  | DA    | 896     | A    | 7.5  |
| 39  | BQ    | 141     | GLN  | 7.4  |
| 48  | DZ    | 176     | PRO  | 7.3  |
| 28  | DB    | 88      | C    | 7.3  |
| 27  | DA    | 2801(A) | A    | 7.3  |
| 7   | AG    | 83      | ALA  | 7.3  |
| 27  | DA    | 2796    | U    | 7.2  |
| 29  | DC    | 166     | ASP  | 7.0  |
| 34  | DH    | 43      | VAL  | 7.0  |
| 29  | DC    | 77      | ILE  | 7.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | CY           | 57         | A           | 7.0         |
| 29         | DC           | 135        | GLY         | 7.0         |
| 27         | BA           | 2799       | C           | 6.9         |
| 29         | BC           | 91         | ALA         | 6.9         |
| 29         | BC           | 176        | GLY         | 6.8         |
| 43         | BU           | 118        | GLY         | 6.8         |
| 48         | BZ           | 175        | PRO         | 6.7         |
| 29         | BC           | 92         | ASP         | 6.7         |
| 21         | AU           | 17         | THR         | 6.7         |
| 21         | AU           | 19         | GLY         | 6.6         |
| 29         | BC           | 121        | GLY         | 6.6         |
| 48         | BZ           | 176        | PRO         | 6.5         |
| 29         | BC           | 77         | ILE         | 6.5         |
| 47         | BY           | 52         | SER         | 6.5         |
| 55         | B6           | 42         | TRP         | 6.5         |
| 42         | BT           | 138        | ALA         | 6.4         |
| 29         | BC           | 43         | VAL         | 6.3         |
| 48         | DZ           | 174        | VAL         | 6.3         |
| 27         | DA           | 2169       | A           | 6.3         |
| 29         | BC           | 132        | GLY         | 6.2         |
| 29         | DC           | 153        | ILE         | 6.2         |
| 41         | DS           | 37         | ALA         | 6.1         |
| 21         | CU           | 18         | TYR         | 6.1         |
| 1          | CA           | 1030(B)    | C           | 6.0         |
| 34         | DH           | 170        | ARG         | 6.0         |
| 11         | AK           | 129        | SER         | 6.0         |
| 25         | AY           | 19         | U           | 6.0         |
| 34         | DH           | 96         | ALA         | 6.0         |
| 29         | BC           | 84         | LYS         | 6.0         |
| 29         | DC           | 95         | GLY         | 5.9         |
| 1          | CA           | 1030(A)    | G           | 5.9         |
| 20         | CT           | 104        | LEU         | 5.9         |
| 48         | DZ           | 110        | VAL         | 5.9         |
| 21         | CU           | 17         | THR         | 5.9         |
| 7          | AG           | 82         | GLY         | 5.8         |
| 1          | CA           | 1027       | C           | 5.8         |
| 19         | CS           | 36         | ARG         | 5.8         |
| 25         | AY           | 17         | G           | 5.8         |
| 29         | DC           | 163        | PHE         | 5.8         |
| 54         | D5           | 2          | ALA         | 5.7         |
| 25         | CY           | 33         | G           | 5.7         |
| 55         | D6           | 42         | TRP         | 5.7         |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 27  | DA    | 2794    | C    | 5.7  |
| 27  | DA    | 2125    | G    | 5.7  |
| 27  | DA    | 2893    | G    | 5.6  |
| 29  | DC    | 57      | ASN  | 5.6  |
| 34  | DH    | 52      | VAL  | 5.6  |
| 19  | AS    | 81      | ARG  | 5.5  |
| 27  | DA    | 2894    | G    | 5.5  |
| 52  | D3    | 1       | MET  | 5.5  |
| 10  | CJ    | 10      | GLY  | 5.4  |
| 25  | AY    | 60      | C    | 5.4  |
| 34  | DH    | 169     | VAL  | 5.4  |
| 29  | DC    | 148     | ASN  | 5.4  |
| 29  | DC    | 96      | GLY  | 5.4  |
| 19  | CS    | 81      | ARG  | 5.3  |
| 21  | CU    | 24      | ARG  | 5.3  |
| 29  | DC    | 72      | VAL  | 5.3  |
| 31  | BE    | 205     | ALA  | 5.3  |
| 29  | DC    | 140     | PRO  | 5.3  |
| 33  | DG    | 89      | GLY  | 5.3  |
| 23  | AW    | 15      | G    | 5.3  |
| 27  | DA    | 2803    | C    | 5.3  |
| 48  | BZ    | 174     | VAL  | 5.2  |
| 27  | DA    | 1044    | G    | 5.2  |
| 48  | BZ    | 169     | THR  | 5.2  |
| 29  | DC    | 37      | PHE  | 5.2  |
| 29  | BC    | 110     | PHE  | 5.2  |
| 42  | DT    | 116     | ALA  | 5.1  |
| 48  | DZ    | 96      | GLU  | 5.1  |
| 25  | CY    | 48      | C    | 5.1  |
| 25  | CY    | 55      | C    | 5.0  |
| 29  | BC    | 74      | VAL  | 5.0  |
| 55  | B6    | 20      | ASN  | 5.0  |
| 27  | BA    | 2801(A) | A    | 5.0  |
| 25  | CY    | 32      | U    | 5.0  |
| 48  | DZ    | 114     | GLY  | 4.9  |
| 47  | DY    | 51      | VAL  | 4.9  |
| 48  | BZ    | 143     | LEU  | 4.9  |
| 29  | BC    | 76      | ALA  | 4.9  |
| 29  | DC    | 35      | ALA  | 4.9  |
| 1   | CA    | 1030(C) | G    | 4.9  |
| 29  | DC    | 76      | ALA  | 4.9  |
| 25  | CY    | 54      | U    | 4.9  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | AY           | 58         | A           | 4.9         |
| 29         | DC           | 70         | LYS         | 4.8         |
| 52         | B3           | 1          | MET         | 4.8         |
| 16         | CP           | 84         | ALA         | 4.8         |
| 29         | BC           | 119        | VAL         | 4.8         |
| 1          | CA           | 1001(A)    | G           | 4.8         |
| 29         | BC           | 89         | ALA         | 4.8         |
| 42         | DT           | 117        | ASP         | 4.8         |
| 25         | CY           | 58         | A           | 4.8         |
| 25         | AY           | 35         | G           | 4.7         |
| 12         | CL           | 126        | ALA         | 4.7         |
| 19         | CS           | 34         | TRP         | 4.7         |
| 27         | BA           | 2173       | A           | 4.7         |
| 1          | AA           | 1036       | G           | 4.7         |
| 48         | BZ           | 96         | GLU         | 4.7         |
| 29         | DC           | 79         | LYS         | 4.7         |
| 29         | DC           | 151        | GLU         | 4.7         |
| 42         | DT           | 2          | ASN         | 4.7         |
| 25         | CY           | 34         | U           | 4.7         |
| 11         | CK           | 42         | TRP         | 4.7         |
| 27         | BA           | 2796       | U           | 4.7         |
| 31         | BE           | 204        | ALA         | 4.7         |
| 7          | CG           | 78         | ARG         | 4.6         |
| 7          | CG           | 82         | GLY         | 4.6         |
| 9          | AI           | 4          | TYR         | 4.6         |
| 48         | BZ           | 178        | ASP         | 4.6         |
| 49         | D0           | 12         | ASN         | 4.6         |
| 2          | CB           | 133        | LYS         | 4.6         |
| 10         | AJ           | 71         | LEU         | 4.6         |
| 23         | AW           | 49         | G           | 4.6         |
| 29         | BC           | 52         | ARG         | 4.6         |
| 27         | BA           | 896        | A           | 4.6         |
| 27         | DA           | 2173       | A           | 4.6         |
| 29         | DC           | 217        | THR         | 4.6         |
| 34         | DH           | 134        | SER         | 4.6         |
| 23         | AW           | 13         | A           | 4.6         |
| 19         | CS           | 82         | GLY         | 4.6         |
| 49         | D0           | 13         | GLY         | 4.5         |
| 38         | BP           | 149        | GLU         | 4.5         |
| 1          | AA           | 1028       | C           | 4.5         |
| 25         | AY           | 7          | A           | 4.5         |
| 29         | BC           | 139        | ASN         | 4.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 15         | CO           | 89         | GLY         | 4.4         |
| 29         | BC           | 72         | VAL         | 4.4         |
| 25         | CY           | 7          | A           | 4.4         |
| 19         | CS           | 37         | ARG         | 4.4         |
| 1          | AA           | 1026       | G           | 4.4         |
| 11         | CK           | 11         | LYS         | 4.4         |
| 1          | CA           | 1024       | G           | 4.4         |
| 29         | BC           | 88         | GLU         | 4.4         |
| 48         | BZ           | 111        | ARG         | 4.4         |
| 9          | AI           | 7          | THR         | 4.4         |
| 29         | DC           | 87         | GLU         | 4.4         |
| 29         | DC           | 92         | ASP         | 4.3         |
| 27         | DA           | 883        | G           | 4.3         |
| 24         | AX           | 1          | C           | 4.3         |
| 27         | DA           | 2155       | G           | 4.3         |
| 29         | DC           | 93         | TYR         | 4.3         |
| 27         | BA           | 2116       | G           | 4.3         |
| 29         | BC           | 79         | LYS         | 4.3         |
| 29         | BC           | 109        | ASP         | 4.3         |
| 43         | DU           | 89         | GLU         | 4.3         |
| 25         | AY           | 48         | C           | 4.3         |
| 28         | BB           | 88         | C           | 4.3         |
| 27         | DA           | 2801       | A           | 4.3         |
| 38         | DP           | 150        | ALA         | 4.3         |
| 21         | CU           | 22         | ARG         | 4.2         |
| 48         | DZ           | 126        | LYS         | 4.2         |
| 23         | AW           | 45         | U           | 4.2         |
| 29         | BC           | 78         | ALA         | 4.2         |
| 33         | DG           | 41         | GLN         | 4.2         |
| 29         | DC           | 182        | PRO         | 4.2         |
| 4          | AD           | 134        | ASP         | 4.2         |
| 29         | DC           | 136        | LEU         | 4.2         |
| 1          | CA           | 1026       | G           | 4.2         |
| 9          | CI           | 4          | TYR         | 4.2         |
| 27         | BA           | 2793       | G           | 4.1         |
| 23         | AW           | 14         | A           | 4.1         |
| 48         | DZ           | 143        | LEU         | 4.1         |
| 25         | AY           | 46         | U           | 4.1         |
| 25         | AY           | 20         | A           | 4.1         |
| 25         | AY           | 47         | C           | 4.1         |
| 19         | CS           | 12         | ASP         | 4.1         |
| 10         | AJ           | 10         | GLY         | 4.1         |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 20  | AT    | 103     | GLY  | 4.1  |
| 11  | CK    | 32      | ILE  | 4.1  |
| 29  | DC    | 78      | ALA  | 4.1  |
| 27  | DA    | 2174    | C    | 4.1  |
| 25  | CY    | 46      | U    | 4.1  |
| 29  | DC    | 177     | LYS  | 4.1  |
| 1   | CA    | 1442(A) | G    | 4.1  |
| 48  | DZ    | 95      | VAL  | 4.0  |
| 27  | BA    | 2151    | G    | 4.0  |
| 3   | CC    | 155     | GLY  | 4.0  |
| 54  | B5    | 60      | VAL  | 4.0  |
| 25  | CY    | 47      | C    | 4.0  |
| 27  | BA    | 884     | C    | 4.0  |
| 9   | CI    | 19      | LEU  | 4.0  |
| 10  | AJ    | 86      | MET  | 4.0  |
| 54  | D5    | 59      | GLU  | 4.0  |
| 47  | DY    | 52      | SER  | 4.0  |
| 22  | AV    | 1       | A    | 4.0  |
| 10  | CJ    | 75      | ILE  | 4.0  |
| 11  | CK    | 89      | ALA  | 4.0  |
| 47  | DY    | 50      | ARG  | 4.0  |
| 25  | CY    | 17      | G    | 3.9  |
| 27  | BA    | 2174    | C    | 3.9  |
| 2   | AB    | 7       | VAL  | 3.9  |
| 1   | CA    | 1036    | G    | 3.9  |
| 33  | DG    | 74      | LYS  | 3.9  |
| 29  | DC    | 80      | GLY  | 3.9  |
| 23  | CW    | 49      | G    | 3.9  |
| 25  | CY    | 18      | G    | 3.9  |
| 25  | AY    | 57      | A    | 3.9  |
| 29  | DC    | 90      | GLY  | 3.9  |
| 49  | D0    | 14      | ARG  | 3.9  |
| 48  | DZ    | 113     | GLY  | 3.9  |
| 48  | BZ    | 106     | THR  | 3.9  |
| 27  | DA    | 888     | C    | 3.9  |
| 29  | DC    | 34      | THR  | 3.9  |
| 27  | BA    | 2803    | C    | 3.8  |
| 29  | BC    | 93      | TYR  | 3.8  |
| 29  | DC    | 69      | GLY  | 3.8  |
| 29  | BC    | 133     | PRO  | 3.8  |
| 2   | CB    | 222     | ILE  | 3.8  |
| 44  | DV    | 38      | LEU  | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 43  | DU    | 90   | VAL  | 3.8  |
| 19  | AS    | 33   | THR  | 3.8  |
| 42  | BT    | 39   | ARG  | 3.8  |
| 34  | DH    | 34   | GLU  | 3.8  |
| 42  | BT    | 137  | LYS  | 3.8  |
| 2   | AB    | 133  | LYS  | 3.7  |
| 10  | CJ    | 72   | VAL  | 3.7  |
| 29  | DC    | 40   | THR  | 3.7  |
| 27  | BA    | 652  | C    | 3.7  |
| 43  | DU    | 91   | ASP  | 3.7  |
| 58  | D9    | 5    | ALA  | 3.7  |
| 29  | DC    | 119  | VAL  | 3.7  |
| 3   | CC    | 189  | ALA  | 3.7  |
| 27  | DA    | 11   | G    | 3.7  |
| 12  | CL    | 65   | ALA  | 3.7  |
| 48  | DZ    | 117  | GLN  | 3.7  |
| 27  | DA    | 2892 | A    | 3.7  |
| 15  | AO    | 89   | GLY  | 3.7  |
| 42  | BT    | 1    | MET  | 3.7  |
| 41  | DS    | 36   | TYR  | 3.7  |
| 1   | AA    | 91   | C    | 3.7  |
| 25  | AY    | 49   | G    | 3.7  |
| 29  | BC    | 40   | THR  | 3.7  |
| 48  | DZ    | 161  | GLU  | 3.7  |
| 23  | CW    | 48   | C    | 3.7  |
| 11  | CK    | 22   | HIS  | 3.7  |
| 9   | AI    | 6    | GLY  | 3.6  |
| 49  | D0    | 11   | ARG  | 3.6  |
| 34  | DH    | 40   | GLU  | 3.6  |
| 25  | AY    | 33   | G    | 3.6  |
| 1   | AA    | 1005 | A    | 3.6  |
| 33  | BG    | 2    | PRO  | 3.6  |
| 33  | BG    | 71   | THR  | 3.6  |
| 51  | B2    | 71   | ASN  | 3.6  |
| 58  | D9    | 24   | TYR  | 3.6  |
| 29  | BC    | 38   | ASP  | 3.6  |
| 10  | AJ    | 98   | ILE  | 3.6  |
| 27  | DA    | 1055 | G    | 3.6  |
| 1   | CA    | 1043 | C    | 3.6  |
| 3   | CC    | 60   | ALA  | 3.6  |
| 2   | AB    | 40   | HIS  | 3.6  |
| 20  | CT    | 103  | GLY  | 3.6  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 29  | BC    | 81      | GLU  | 3.6  |
| 54  | D5    | 60      | VAL  | 3.6  |
| 14  | CN    | 2       | ALA  | 3.6  |
| 23  | CW    | 16      | C    | 3.5  |
| 25  | CY    | 49      | G    | 3.5  |
| 1   | AA    | 1030(C) | G    | 3.5  |
| 27  | BA    | 2894    | G    | 3.5  |
| 29  | BC    | 83      | ILE  | 3.5  |
| 29  | DC    | 99      | ILE  | 3.5  |
| 51  | B2    | 72      | ALA  | 3.5  |
| 29  | DC    | 62      | VAL  | 3.5  |
| 48  | DZ    | 26      | VAL  | 3.5  |
| 58  | D9    | 37      | GLY  | 3.5  |
| 27  | DA    | 1047    | G    | 3.5  |
| 29  | DC    | 180     | PHE  | 3.5  |
| 48  | DZ    | 87      | PHE  | 3.5  |
| 42  | DT    | 137     | LYS  | 3.5  |
| 34  | DH    | 44      | VAL  | 3.5  |
| 48  | DZ    | 97      | MET  | 3.5  |
| 29  | DC    | 58      | VAL  | 3.5  |
| 29  | BC    | 148     | ASN  | 3.4  |
| 25  | CY    | 59      | U    | 3.4  |
| 27  | DA    | 2793    | G    | 3.4  |
| 12  | CL    | 53      | ALA  | 3.4  |
| 34  | DH    | 19      | VAL  | 3.4  |
| 42  | BT    | 93      | ARG  | 3.4  |
| 1   | AA    | 1031    | G    | 3.4  |
| 29  | BC    | 86      | ALA  | 3.4  |
| 27  | BA    | 2156    | G    | 3.4  |
| 27  | BA    | 897     | C    | 3.4  |
| 42  | DT    | 115     | ARG  | 3.4  |
| 27  | BA    | 2804    | C    | 3.4  |
| 29  | BC    | 108     | MET  | 3.4  |
| 13  | CM    | 101     | GLN  | 3.4  |
| 29  | DC    | 71      | GLN  | 3.4  |
| 27  | BA    | 2794    | C    | 3.4  |
| 29  | BC    | 53      | ARG  | 3.4  |
| 48  | DZ    | 107     | PRO  | 3.4  |
| 11  | CK    | 13      | GLN  | 3.4  |
| 13  | AM    | 6       | GLY  | 3.4  |
| 25  | CY    | 20      | A    | 3.3  |
| 19  | AS    | 52      | TYR  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | CU    | 25   | LYS  | 3.3  |
| 16  | AP    | 13   | HIS  | 3.3  |
| 43  | DU    | 117  | GLN  | 3.3  |
| 48  | DZ    | 93   | GLU  | 3.3  |
| 7   | CG    | 84   | ASN  | 3.3  |
| 33  | DG    | 75   | LYS  | 3.3  |
| 55  | B6    | 21   | TYR  | 3.3  |
| 31  | DE    | 35   | GLN  | 3.3  |
| 11  | CK    | 129  | SER  | 3.3  |
| 29  | BC    | 180  | PHE  | 3.3  |
| 3   | CC    | 2    | GLY  | 3.3  |
| 49  | B0    | 8    | GLY  | 3.3  |
| 29  | BC    | 141  | LYS  | 3.3  |
| 48  | DZ    | 71   | ARG  | 3.3  |
| 27  | BA    | 878  | A    | 3.3  |
| 29  | DC    | 74   | VAL  | 3.3  |
| 27  | DA    | 2154 | G    | 3.3  |
| 32  | DF    | 1    | MET  | 3.3  |
| 48  | BZ    | 112  | ALA  | 3.3  |
| 29  | DC    | 84   | LYS  | 3.3  |
| 32  | BF    | 2    | LYS  | 3.3  |
| 2   | CB    | 32   | ILE  | 3.3  |
| 52  | D3    | 29   | ARG  | 3.3  |
| 49  | D0    | 41   | ARG  | 3.2  |
| 1   | CA    | 1025 | U    | 3.2  |
| 29  | BC    | 42   | GLU  | 3.2  |
| 42  | DT    | 122  | ASP  | 3.2  |
| 1   | CA    | 1034 | G    | 3.2  |
| 7   | CG    | 86   | GLN  | 3.2  |
| 23  | AW    | 46   | U    | 3.2  |
| 25  | CY    | 60   | C    | 3.2  |
| 1   | AA    | 1025 | U    | 3.2  |
| 2   | CB    | 233  | SER  | 3.2  |
| 16  | AP    | 12   | LYS  | 3.2  |
| 19  | AS    | 56   | GLN  | 3.2  |
| 27  | DA    | 2156 | G    | 3.2  |
| 10  | CJ    | 39   | PRO  | 3.2  |
| 42  | DT    | 138  | ALA  | 3.2  |
| 27  | BA    | 2896 | C    | 3.2  |
| 2   | CB    | 215  | LEU  | 3.2  |
| 19  | CS    | 69   | HIS  | 3.2  |
| 29  | BC    | 37   | PHE  | 3.2  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 29  | BC    | 154     | ARG  | 3.2  |
| 27  | BA    | 1048    | A    | 3.2  |
| 42  | DT    | 119     | LYS  | 3.2  |
| 13  | AM    | 102     | ARG  | 3.2  |
| 27  | DA    | 2310    | A    | 3.2  |
| 29  | DC    | 164     | ARG  | 3.2  |
| 2   | AB    | 20      | GLU  | 3.2  |
| 35  | DI    | 23      | PRO  | 3.2  |
| 50  | D1    | 81      | LYS  | 3.2  |
| 19  | AS    | 82      | GLY  | 3.1  |
| 32  | DF    | 11      | VAL  | 3.1  |
| 19  | CS    | 38      | SER  | 3.1  |
| 14  | CN    | 4       | LYS  | 3.1  |
| 29  | DC    | 66      | HIS  | 3.1  |
| 23  | AW    | 9       | C    | 3.1  |
| 21  | AU    | 5       | ASP  | 3.1  |
| 1   | AA    | 1030(D) | A    | 3.1  |
| 7   | CG    | 4       | ARG  | 3.1  |
| 29  | DC    | 38      | ASP  | 3.1  |
| 29  | DC    | 134     | ARG  | 3.1  |
| 21  | CU    | 23      | PRO  | 3.1  |
| 27  | BA    | 1044    | G    | 3.1  |
| 27  | DA    | 275     | G    | 3.1  |
| 27  | DA    | 2127    | G    | 3.1  |
| 34  | DH    | 123     | PHE  | 3.1  |
| 27  | BA    | 2136    | C    | 3.1  |
| 29  | BC    | 94      | VAL  | 3.1  |
| 55  | D6    | 39      | TYR  | 3.1  |
| 9   | AI    | 9       | ARG  | 3.1  |
| 27  | BA    | 2126    | A    | 3.1  |
| 25  | AY    | 15      | G    | 3.1  |
| 29  | DC    | 154     | ARG  | 3.1  |
| 48  | BZ    | 97      | MET  | 3.1  |
| 29  | BC    | 65      | PRO  | 3.1  |
| 2   | AB    | 11      | LEU  | 3.1  |
| 48  | BZ    | 172     | ALA  | 3.1  |
| 1   | CA    | 91      | C    | 3.1  |
| 29  | BC    | 134     | ARG  | 3.1  |
| 1   | CA    | 1094    | G    | 3.1  |
| 20  | AT    | 83      | ARG  | 3.1  |
| 48  | DZ    | 77      | LYS  | 3.1  |
| 28  | DB    | 87      | G    | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | CG    | 3    | ARG  | 3.1  |
| 1   | AA    | 1024 | G    | 3.0  |
| 12  | CL    | 125  | ALA  | 3.0  |
| 1   | AA    | 76   | C    | 3.0  |
| 27  | BA    | 275  | G    | 3.0  |
| 33  | BG    | 88   | ILE  | 3.0  |
| 4   | CD    | 209  | ARG  | 3.0  |
| 27  | BA    | 2141 | G    | 3.0  |
| 27  | DA    | 2124 | G    | 3.0  |
| 23  | CW    | 10   | G    | 3.0  |
| 21  | AU    | 18   | TYR  | 3.0  |
| 29  | BC    | 44   | HIS  | 3.0  |
| 54  | D5    | 58   | LEU  | 3.0  |
| 11  | AK    | 95   | ILE  | 3.0  |
| 48  | BZ    | 168  | GLU  | 3.0  |
| 54  | B5    | 2    | ALA  | 3.0  |
| 29  | DC    | 61   | THR  | 3.0  |
| 27  | DA    | 2791 | C    | 3.0  |
| 27  | DA    | 1046 | A    | 3.0  |
| 48  | DZ    | 146  | GLY  | 3.0  |
| 15  | AO    | 87   | ILE  | 3.0  |
| 48  | DZ    | 140  | VAL  | 3.0  |
| 48  | DZ    | 173  | VAL  | 3.0  |
| 42  | DT    | 40   | THR  | 3.0  |
| 29  | BC    | 174  | PRO  | 3.0  |
| 21  | AU    | 2    | GLY  | 3.0  |
| 7   | AG    | 4    | ARG  | 3.0  |
| 13  | CM    | 84   | ILE  | 3.0  |
| 23  | AW    | 16   | C    | 3.0  |
| 1   | CA    | 1005 | A    | 3.0  |
| 49  | D0    | 10   | THR  | 3.0  |
| 55  | D6    | 40   | CYS  | 3.0  |
| 27  | BA    | 2127 | G    | 2.9  |
| 21  | AU    | 21   | TYR  | 2.9  |
| 44  | DV    | 5    | VAL  | 2.9  |
| 29  | BC    | 87   | GLU  | 2.9  |
| 29  | BC    | 216  | THR  | 2.9  |
| 29  | DC    | 181  | PRO  | 2.9  |
| 11  | AK    | 14   | VAL  | 2.9  |
| 27  | DA    | 2152 | G    | 2.9  |
| 29  | DC    | 159  | GLY  | 2.9  |
| 7   | AG    | 79   | ARG  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | DC    | 97   | GLU  | 2.9  |
| 4   | AD    | 7    | PRO  | 2.9  |
| 10  | AJ    | 85   | LEU  | 2.9  |
| 58  | D9    | 25   | VAL  | 2.9  |
| 15  | AO    | 88   | ARG  | 2.9  |
| 1   | CA    | 1031 | G    | 2.9  |
| 1   | CA    | 1117 | G    | 2.9  |
| 23  | CW    | 50   | A    | 2.9  |
| 29  | DC    | 73   | ARG  | 2.9  |
| 27  | DA    | 897  | C    | 2.9  |
| 29  | DC    | 187  | ASP  | 2.9  |
| 8   | CH    | 55   | GLY  | 2.9  |
| 10  | CJ    | 85   | LEU  | 2.9  |
| 1   | AA    | 1129 | C    | 2.9  |
| 1   | AA    | 104  | G    | 2.9  |
| 9   | AI    | 18   | PHE  | 2.9  |
| 16  | AP    | 11   | SER  | 2.9  |
| 27  | DA    | 2792 | G    | 2.9  |
| 38  | DP    | 118  | GLY  | 2.9  |
| 29  | BC    | 131  | LEU  | 2.9  |
| 58  | D9    | 34   | GLN  | 2.9  |
| 9   | CI    | 62   | TYR  | 2.9  |
| 42  | DT    | 36   | GLU  | 2.9  |
| 27  | BA    | 2138 | C    | 2.9  |
| 48  | BZ    | 148  | SER  | 2.9  |
| 23  | AW    | 50   | A    | 2.9  |
| 34  | DH    | 23   | ARG  | 2.9  |
| 58  | D9    | 26   | ILE  | 2.8  |
| 25  | AY    | 18   | G    | 2.8  |
| 42  | DT    | 92   | GLY  | 2.8  |
| 11  | AK    | 28   | THR  | 2.8  |
| 29  | DC    | 192  | PHE  | 2.8  |
| 56  | D7    | 23   | ARG  | 2.8  |
| 41  | DS    | 47   | THR  | 2.8  |
| 5   | AE    | 91   | LEU  | 2.8  |
| 15  | AO    | 67   | LEU  | 2.8  |
| 23  | AW    | 8    | U    | 2.8  |
| 43  | DU    | 118  | GLY  | 2.8  |
| 34  | BH    | 136  | ILE  | 2.8  |
| 33  | DG    | 43   | LEU  | 2.8  |
| 25  | AY    | 16   | C    | 2.8  |
| 1   | AA    | 1286 | A    | 2.8  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | CA    | 1225    | A    | 2.8  |
| 1   | CA    | 1003    | G    | 2.8  |
| 27  | BA    | 2150    | U    | 2.8  |
| 47  | DY    | 55      | TYR  | 2.8  |
| 41  | DS    | 30      | ARG  | 2.8  |
| 23  | AW    | 48      | C    | 2.8  |
| 28  | DB    | 6       | C    | 2.8  |
| 4   | AD    | 209     | ARG  | 2.8  |
| 7   | AG    | 85      | TYR  | 2.8  |
| 50  | B1    | 82      | LEU  | 2.8  |
| 9   | CI    | 18      | PHE  | 2.8  |
| 27  | DA    | 2137    | C    | 2.8  |
| 29  | BC    | 177     | LYS  | 2.8  |
| 57  | D8    | 65      | GLU  | 2.8  |
| 29  | BC    | 107     | TRP  | 2.8  |
| 33  | DG    | 182     | LYS  | 2.8  |
| 25  | AY    | 64      | G    | 2.8  |
| 48  | DZ    | 11      | GLY  | 2.8  |
| 48  | DZ    | 105     | GLY  | 2.8  |
| 43  | DU    | 88      | ILE  | 2.8  |
| 31  | DE    | 205     | ALA  | 2.8  |
| 47  | DY    | 59      | GLY  | 2.8  |
| 1   | CA    | 1030    | C    | 2.8  |
| 27  | DA    | 2138    | C    | 2.8  |
| 29  | DC    | 147     | PHE  | 2.8  |
| 55  | D6    | 41      | PRO  | 2.8  |
| 29  | DC    | 161     | ILE  | 2.7  |
| 1   | AA    | 1030(A) | G    | 2.7  |
| 2   | AB    | 136     | VAL  | 2.7  |
| 12  | CL    | 67      | ILE  | 2.7  |
| 30  | BD    | 244     | ARG  | 2.7  |
| 27  | BA    | 2155    | G    | 2.7  |
| 10  | AJ    | 23      | ILE  | 2.7  |
| 55  | D6    | 20      | ASN  | 2.7  |
| 18  | AR    | 31      | LEU  | 2.7  |
| 27  | BA    | 2402    | C    | 2.7  |
| 44  | BV    | 48      | GLY  | 2.7  |
| 10  | AJ    | 69      | ASN  | 2.7  |
| 27  | DA    | 2139    | C    | 2.7  |
| 29  | DC    | 88      | GLU  | 2.7  |
| 19  | AS    | 71      | LEU  | 2.7  |
| 27  | BA    | 352     | G    | 2.7  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 27         | DA           | 271(A)     | A           | 2.7         |
| 27         | DA           | 2348       | U           | 2.7         |
| 33         | DG           | 4          | ASP         | 2.7         |
| 43         | DU           | 79         | PHE         | 2.7         |
| 48         | BZ           | 177        | GLU         | 2.7         |
| 19         | CS           | 35         | SER         | 2.7         |
| 34         | DH           | 56         | SER         | 2.7         |
| 29         | BC           | 106        | GLY         | 2.7         |
| 42         | BT           | 115        | ARG         | 2.7         |
| 56         | D7           | 29         | LYS         | 2.7         |
| 29         | BC           | 18         | LYS         | 2.7         |
| 19         | AS           | 77         | THR         | 2.7         |
| 21         | CU           | 13         | ILE         | 2.7         |
| 27         | DA           | 1108       | U           | 2.7         |
| 31         | DE           | 204        | ALA         | 2.7         |
| 27         | BA           | 2131       | G           | 2.7         |
| 27         | DA           | 1052       | C           | 2.7         |
| 49         | B0           | 7          | LEU         | 2.7         |
| 33         | BG           | 178        | PHE         | 2.7         |
| 27         | BA           | 2130       | U           | 2.7         |
| 27         | DA           | 1045       | A           | 2.7         |
| 27         | DA           | 1048       | A           | 2.7         |
| 25         | AY           | 63         | C           | 2.7         |
| 44         | DV           | 36         | PRO         | 2.7         |
| 9          | AI           | 102        | LEU         | 2.6         |
| 20         | CT           | 102        | GLY         | 2.6         |
| 33         | DG           | 40         | ASN         | 2.6         |
| 11         | CK           | 90         | GLY         | 2.6         |
| 21         | AU           | 25         | LYS         | 2.6         |
| 43         | DU           | 69         | CYS         | 2.6         |
| 38         | BP           | 150        | ALA         | 2.6         |
| 27         | DA           | 1049       | C           | 2.6         |
| 48         | BZ           | 87         | PHE         | 2.6         |
| 2          | CB           | 203        | GLY         | 2.6         |
| 8          | CH           | 1          | MET         | 2.6         |
| 29         | BC           | 75         | LEU         | 2.6         |
| 38         | DP           | 51         | PHE         | 2.6         |
| 56         | D7           | 18         | PHE         | 2.6         |
| 11         | AK           | 81         | ASP         | 2.6         |
| 4          | AD           | 3          | ARG         | 2.6         |
| 34         | DH           | 105        | LEU         | 2.6         |
| 23         | AW           | 10         | G           | 2.6         |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 27  | BA    | 1176   | G    | 2.6  |
| 38  | BP    | 15     | ARG  | 2.6  |
| 28  | BB    | 87     | G    | 2.6  |
| 35  | DI    | 24     | GLY  | 2.6  |
| 2   | AB    | 163    | PHE  | 2.6  |
| 29  | DC    | 132    | GLY  | 2.6  |
| 21  | CU    | 9      | ARG  | 2.6  |
| 27  | DA    | 271(G) | C    | 2.6  |
| 33  | BG    | 182    | LYS  | 2.6  |
| 29  | DC    | 43     | VAL  | 2.6  |
| 48  | DZ    | 115    | VAL  | 2.6  |
| 2   | CB    | 232    | PRO  | 2.6  |
| 3   | CC    | 196    | LEU  | 2.6  |
| 11  | AK    | 29     | ILE  | 2.6  |
| 1   | CA    | 993    | G    | 2.5  |
| 1   | CA    | 1042   | G    | 2.5  |
| 25  | CY    | 56     | G    | 2.5  |
| 29  | BC    | 95     | GLY  | 2.5  |
| 2   | AB    | 214    | ILE  | 2.5  |
| 32  | DF    | 10     | PRO  | 2.5  |
| 48  | DZ    | 132    | ILE  | 2.5  |
| 29  | BC    | 73     | ARG  | 2.5  |
| 48  | DZ    | 142    | GLY  | 2.5  |
| 19  | AS    | 57     | HIS  | 2.5  |
| 27  | DA    | 1053   | C    | 2.5  |
| 29  | DC    | 39     | GLU  | 2.5  |
| 27  | DA    | 2123   | G    | 2.5  |
| 10  | CJ    | 74     | ILE  | 2.5  |
| 57  | B8    | 65     | GLU  | 2.5  |
| 27  | BA    | 2137   | C    | 2.5  |
| 31  | DE    | 186    | GLY  | 2.5  |
| 50  | D1    | 33     | LYS  | 2.5  |
| 1   | AA    | 70     | G    | 2.5  |
| 2   | CB    | 41     | ILE  | 2.5  |
| 17  | AQ    | 71     | PHE  | 2.5  |
| 2   | AB    | 232    | PRO  | 2.5  |
| 48  | DZ    | 108    | ALA  | 2.5  |
| 41  | DS    | 39     | ILE  | 2.5  |
| 29  | DC    | 89     | ALA  | 2.5  |
| 1   | AA    | 841    | U    | 2.5  |
| 25  | CY    | 31     | U    | 2.5  |
| 32  | DF    | 169    | ASN  | 2.5  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 3   | AC    | 182     | ILE  | 2.5  |
| 20  | CT    | 60      | GLU  | 2.5  |
| 21  | CU    | 12      | LYS  | 2.5  |
| 33  | DG    | 137     | GLU  | 2.5  |
| 10  | AJ    | 72      | VAL  | 2.5  |
| 20  | AT    | 80      | ARG  | 2.5  |
| 34  | DH    | 24      | VAL  | 2.5  |
| 48  | DZ    | 94      | PRO  | 2.5  |
| 1   | CA    | 69      | G    | 2.5  |
| 34  | DH    | 41      | MET  | 2.5  |
| 3   | CC    | 197     | GLY  | 2.5  |
| 1   | AA    | 1030(B) | C    | 2.5  |
| 33  | BG    | 86      | MET  | 2.5  |
| 11  | CK    | 31      | THR  | 2.5  |
| 29  | BC    | 190     | ARG  | 2.5  |
| 9   | AI    | 15      | ALA  | 2.5  |
| 27  | BA    | 2125    | G    | 2.5  |
| 29  | BC    | 19      | VAL  | 2.5  |
| 55  | D6    | 21      | TYR  | 2.5  |
| 29  | BC    | 149     | ILE  | 2.5  |
| 29  | BC    | 155     | GLU  | 2.5  |
| 34  | BH    | 169     | VAL  | 2.5  |
| 44  | DV    | 33      | VAL  | 2.5  |
| 2   | CB    | 106     | LYS  | 2.5  |
| 1   | AA    | 77      | G    | 2.5  |
| 9   | CI    | 20      | ARG  | 2.5  |
| 21  | CU    | 5       | ASP  | 2.5  |
| 1   | CA    | 1029    | C    | 2.4  |
| 1   | AA    | 1447    | A    | 2.4  |
| 1   | CA    | 1286    | A    | 2.4  |
| 48  | DZ    | 55      | VAL  | 2.4  |
| 47  | DY    | 53      | PRO  | 2.4  |
| 34  | DH    | 124     | GLU  | 2.4  |
| 1   | AA    | 68      | G    | 2.4  |
| 29  | BC    | 41      | VAL  | 2.4  |
| 27  | BA    | 1109    | C    | 2.4  |
| 27  | DA    | 157     | U    | 2.4  |
| 48  | DZ    | 169     | THR  | 2.4  |
| 19  | AS    | 76      | PRO  | 2.4  |
| 21  | AU    | 23      | PRO  | 2.4  |
| 38  | DP    | 117     | GLU  | 2.4  |
| 9   | AI    | 17      | VAL  | 2.4  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 17  | AQ    | 45      | HIS  | 2.4  |
| 38  | BP    | 108     | LYS  | 2.4  |
| 48  | BZ    | 114     | GLY  | 2.4  |
| 21  | AU    | 22      | ARG  | 2.4  |
| 1   | AA    | 1001(A) | G    | 2.4  |
| 24  | CX    | 49      | G    | 2.4  |
| 27  | DA    | 2131    | G    | 2.4  |
| 54  | B5    | 59      | GLU  | 2.4  |
| 3   | CC    | 64      | VAL  | 2.4  |
| 33  | BG    | 43      | LEU  | 2.4  |
| 11  | AK    | 42      | TRP  | 2.4  |
| 55  | D6    | 24      | GLU  | 2.4  |
| 1   | AA    | 1030    | C    | 2.4  |
| 44  | DV    | 94      | LEU  | 2.4  |
| 58  | D9    | 16      | VAL  | 2.4  |
| 27  | DA    | 10      | G    | 2.4  |
| 48  | BZ    | 120     | HIS  | 2.4  |
| 10  | CJ    | 28      | ARG  | 2.4  |
| 20  | AT    | 99      | LEU  | 2.4  |
| 43  | DU    | 83      | LEU  | 2.4  |
| 27  | BA    | 2175    | C    | 2.4  |
| 29  | DC    | 172     | HIS  | 2.4  |
| 38  | BP    | 51      | PHE  | 2.4  |
| 25  | CY    | 51      | G    | 2.4  |
| 27  | BA    | 883     | G    | 2.4  |
| 48  | BZ    | 146     | GLY  | 2.4  |
| 29  | BC    | 166     | ASP  | 2.4  |
| 47  | DY    | 102     | CYS  | 2.4  |
| 41  | DS    | 52      | SER  | 2.4  |
| 1   | AA    | 152     | A    | 2.4  |
| 2   | AB    | 215     | LEU  | 2.4  |
| 7   | AG    | 86      | GLN  | 2.4  |
| 10  | AJ    | 40      | LEU  | 2.4  |
| 11  | AK    | 84      | VAL  | 2.4  |
| 2   | CB    | 37      | ASN  | 2.4  |
| 23  | AW    | 47      | C    | 2.4  |
| 27  | DA    | 899     | A    | 2.4  |
| 58  | D9    | 35      | ARG  | 2.4  |
| 44  | DV    | 96      | ILE  | 2.4  |
| 45  | BW    | 63      | ASP  | 2.4  |
| 2   | CB    | 221     | LEU  | 2.4  |
| 25  | AY    | 34      | U    | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | AM    | 101  | GLN  | 2.4  |
| 34  | DH    | 37   | VAL  | 2.4  |
| 43  | BU    | 117  | GLN  | 2.4  |
| 49  | D0    | 22   | GLY  | 2.4  |
| 29  | DC    | 216  | THR  | 2.4  |
| 25  | AY    | 36   | A    | 2.3  |
| 25  | AY    | 50   | A    | 2.3  |
| 27  | DA    | 2170 | A    | 2.3  |
| 18  | AR    | 88   | LYS  | 2.3  |
| 10  | AJ    | 27   | ALA  | 2.3  |
| 10  | AJ    | 70   | ARG  | 2.3  |
| 11  | AK    | 30   | VAL  | 2.3  |
| 29  | BC    | 165  | ASN  | 2.3  |
| 37  | BO    | 28   | SER  | 2.3  |
| 2   | AB    | 213  | LEU  | 2.3  |
| 48  | DZ    | 90   | LEU  | 2.3  |
| 49  | B0    | 3    | HIS  | 2.3  |
| 36  | DN    | 133  | GLN  | 2.3  |
| 14  | AN    | 32   | SER  | 2.3  |
| 35  | DI    | 72   | LEU  | 2.3  |
| 42  | DT    | 93   | ARG  | 2.3  |
| 43  | DU    | 76   | TYR  | 2.3  |
| 44  | DV    | 39   | LEU  | 2.3  |
| 25  | CY    | 6    | U    | 2.3  |
| 48  | DZ    | 82   | PRO  | 2.3  |
| 2   | CB    | 231  | GLU  | 2.3  |
| 45  | BW    | 60   | ASN  | 2.3  |
| 9   | CI    | 60   | ASP  | 2.3  |
| 21  | AU    | 6    | ARG  | 2.3  |
| 27  | DA    | 919  | G    | 2.3  |
| 44  | DV    | 12   | TYR  | 2.3  |
| 29  | BC    | 102  | LYS  | 2.3  |
| 23  | CW    | 13   | A    | 2.3  |
| 29  | DC    | 158  | ALA  | 2.3  |
| 57  | D8    | 64   | TYR  | 2.3  |
| 34  | DH    | 35   | VAL  | 2.3  |
| 23  | CW    | 15   | G    | 2.3  |
| 24  | CX    | 21   | A    | 2.3  |
| 20  | CT    | 106  | ALA  | 2.3  |
| 12  | CL    | 13   | GLU  | 2.3  |
| 27  | DA    | 894  | C    | 2.3  |
| 4   | AD    | 126  | ILE  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | DC    | 42   | GLU  | 2.3  |
| 24  | AX    | 67   | C    | 2.3  |
| 48  | DZ    | 162  | LEU  | 2.3  |
| 48  | DZ    | 127  | VAL  | 2.3  |
| 21  | CU    | 16   | GLY  | 2.3  |
| 29  | BC    | 80   | GLY  | 2.3  |
| 58  | D9    | 22   | ARG  | 2.3  |
| 5   | AE    | 9    | LYS  | 2.3  |
| 25  | AY    | 52   | G    | 2.3  |
| 43  | DU    | 74   | LEU  | 2.3  |
| 48  | DZ    | 69   | LEU  | 2.3  |
| 2   | CB    | 42   | ILE  | 2.3  |
| 4   | AD    | 4    | TYR  | 2.3  |
| 16  | AP    | 39   | TYR  | 2.3  |
| 21  | CU    | 2    | GLY  | 2.3  |
| 27  | BA    | 1547 | C    | 2.3  |
| 27  | DA    | 2895 | U    | 2.3  |
| 47  | DY    | 46   | LYS  | 2.3  |
| 9   | AI    | 19   | LEU  | 2.3  |
| 33  | DG    | 90   | LEU  | 2.3  |
| 19  | AS    | 39   | THR  | 2.3  |
| 2   | AB    | 38   | GLY  | 2.2  |
| 27  | DA    | 1112 | G    | 2.2  |
| 3   | CC    | 111  | LEU  | 2.2  |
| 27  | BA    | 2897 | U    | 2.2  |
| 34  | DH    | 129  | THR  | 2.2  |
| 1   | CA    | 153  | C    | 2.2  |
| 47  | DY    | 56   | PRO  | 2.2  |
| 10  | CJ    | 20   | ALA  | 2.2  |
| 29  | DC    | 56   | GLN  | 2.2  |
| 41  | DS    | 51   | ALA  | 2.2  |
| 4   | CD    | 134  | ASP  | 2.2  |
| 27  | DA    | 2153 | G    | 2.2  |
| 9   | CI    | 17   | VAL  | 2.2  |
| 13  | CM    | 7    | VAL  | 2.2  |
| 41  | DS    | 49   | VAL  | 2.2  |
| 34  | BH    | 101  | ARG  | 2.2  |
| 29  | BC    | 136  | LEU  | 2.2  |
| 33  | BG    | 90   | LEU  | 2.2  |
| 23  | CW    | 7    | A    | 2.2  |
| 27  | DA    | 1174 | A    | 2.2  |
| 27  | DA    | 1470 | G    | 2.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 34         | BH           | 103        | LEU         | 2.2         |
| 29         | DC           | 100        | ILE         | 2.2         |
| 21         | AU           | 11         | GLY         | 2.2         |
| 32         | DF           | 133        | ASN         | 2.2         |
| 34         | DH           | 128        | PRO         | 2.2         |
| 47         | DY           | 48         | ALA         | 2.2         |
| 27         | DA           | 2151       | G           | 2.2         |
| 2          | AB           | 87         | ARG         | 2.2         |
| 4          | AD           | 133        | VAL         | 2.2         |
| 10         | CJ           | 34         | VAL         | 2.2         |
| 12         | CL           | 36         | VAL         | 2.2         |
| 19         | CS           | 45         | VAL         | 2.2         |
| 41         | DS           | 64         | GLU         | 2.2         |
| 27         | DA           | 181        | A           | 2.2         |
| 32         | BF           | 12         | LEU         | 2.2         |
| 44         | DV           | 22         | VAL         | 2.2         |
| 23         | AW           | 24         | C           | 2.2         |
| 24         | CX           | 7          | G           | 2.2         |
| 33         | BG           | 89         | GLY         | 2.2         |
| 25         | CY           | 44         | U           | 2.2         |
| 23         | CW           | 11         | C           | 2.2         |
| 1          | AA           | 69         | G           | 2.2         |
| 2          | AB           | 190        | THR         | 2.2         |
| 25         | CY           | 52         | G           | 2.2         |
| 27         | DA           | 2141       | G           | 2.2         |
| 29         | BC           | 25         | ALA         | 2.2         |
| 29         | BC           | 189        | ILE         | 2.2         |
| 23         | CW           | 45         | U           | 2.2         |
| 32         | DF           | 167        | ALA         | 2.2         |
| 48         | BZ           | 98         | TYR         | 2.2         |
| 16         | AP           | 41         | PRO         | 2.2         |
| 20         | AT           | 64         | ASP         | 2.2         |
| 47         | BY           | 55         | TYR         | 2.2         |
| 51         | B2           | 51         | ARG         | 2.2         |
| 29         | BC           | 35         | ALA         | 2.2         |
| 1          | AA           | 64         | G           | 2.2         |
| 27         | DA           | 352        | G           | 2.2         |
| 34         | DH           | 81         | GLU         | 2.2         |
| 49         | B0           | 12         | ASN         | 2.2         |
| 30         | BD           | 33         | LEU         | 2.1         |
| 1          | CA           | 92         | C           | 2.1         |
| 10         | AJ           | 6          | ILE         | 2.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | AC    | 87   | LEU  | 2.1  |
| 33  | DG    | 152  | LEU  | 2.1  |
| 29  | DC    | 103  | ILE  | 2.1  |
| 7   | AG    | 81   | GLY  | 2.1  |
| 33  | DG    | 42   | GLY  | 2.1  |
| 29  | BC    | 213  | TYR  | 2.1  |
| 34  | BH    | 102  | ALA  | 2.1  |
| 48  | BZ    | 140  | VAL  | 2.1  |
| 27  | DA    | 884  | C    | 2.1  |
| 3   | AC    | 88   | ARG  | 2.1  |
| 19  | CS    | 70   | LYS  | 2.1  |
| 29  | BC    | 142  | ALA  | 2.1  |
| 10  | CJ    | 82   | ILE  | 2.1  |
| 1   | CA    | 1033 | G    | 2.1  |
| 1   | CA    | 1447 | A    | 2.1  |
| 20  | AT    | 102  | GLY  | 2.1  |
| 27  | BA    | 2310 | A    | 2.1  |
| 28  | DB    | 5    | C    | 2.1  |
| 48  | BZ    | 142  | GLY  | 2.1  |
| 49  | D0    | 7    | LEU  | 2.1  |
| 10  | AJ    | 99   | LYS  | 2.1  |
| 1   | AA    | 391  | G    | 2.1  |
| 3   | AC    | 76   | VAL  | 2.1  |
| 11  | CK    | 30   | VAL  | 2.1  |
| 25  | AY    | 55   | C    | 2.1  |
| 27  | BA    | 888  | C    | 2.1  |
| 27  | BA    | 2139 | C    | 2.1  |
| 27  | DA    | 2142 | C    | 2.1  |
| 49  | D0    | 44   | ARG  | 2.1  |
| 29  | BC    | 182  | PRO  | 2.1  |
| 50  | B1    | 93   | GLU  | 2.1  |
| 1   | CA    | 1001 | A    | 2.1  |
| 27  | DA    | 330  | A    | 2.1  |
| 27  | DA    | 878  | A    | 2.1  |
| 1   | CA    | 1129 | C    | 2.1  |
| 1   | CA    | 1442 | G    | 2.1  |
| 13  | CM    | 103  | THR  | 2.1  |
| 42  | DT    | 38   | ASN  | 2.1  |
| 55  | D6    | 50   | ARG  | 2.1  |
| 41  | DS    | 50   | SER  | 2.1  |
| 11  | AK    | 21   | ILE  | 2.1  |
| 20  | CT    | 101  | GLY  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | BA    | 2805 | G    | 2.1  |
| 27  | DA    | 1042 | G    | 2.1  |
| 27  | DA    | 2157 | G    | 2.1  |
| 42  | DT    | 135  | ALA  | 2.1  |
| 48  | BZ    | 132  | ILE  | 2.1  |
| 9   | CI    | 3    | GLN  | 2.1  |
| 36  | DN    | 77   | GLY  | 2.1  |
| 33  | DG    | 86   | MET  | 2.1  |
| 27  | BA    | 1054 | A    | 2.1  |
| 49  | D0    | 85   | ALA  | 2.1  |
| 11  | AK    | 43   | SER  | 2.1  |
| 42  | DT    | 42   | ILE  | 2.1  |
| 55  | D6    | 46   | HIS  | 2.1  |
| 15  | CO    | 22   | THR  | 2.1  |
| 25  | AY    | 8    | U    | 2.1  |
| 42  | BT    | 36   | GLU  | 2.1  |
| 43  | DU    | 110  | VAL  | 2.1  |
| 20  | CT    | 99   | LEU  | 2.1  |
| 48  | DZ    | 4    | LEU  | 2.1  |
| 23  | AW    | 12   | C    | 2.1  |
| 20  | AT    | 68   | LYS  | 2.0  |
| 56  | D7    | 28   | ARG  | 2.0  |
| 29  | BC    | 215  | THR  | 2.0  |
| 3   | CC    | 158  | GLY  | 2.0  |
| 10  | AJ    | 7    | LYS  | 2.0  |
| 21  | AU    | 24   | ARG  | 2.0  |
| 27  | DA    | 887  | A    | 2.0  |
| 39  | DQ    | 85   | LYS  | 2.0  |
| 4   | AD    | 38   | TYR  | 2.0  |
| 33  | DG    | 159  | VAL  | 2.0  |
| 1   | AA    | 1033 | G    | 2.0  |
| 27  | DA    | 508  | G    | 2.0  |
| 31  | DE    | 48   | GLN  | 2.0  |
| 45  | DW    | 94   | ASP  | 2.0  |
| 29  | BC    | 103  | ILE  | 2.0  |
| 46  | BX    | 92   | LEU  | 2.0  |
| 48  | BZ    | 113  | GLY  | 2.0  |
| 4   | AD    | 125  | HIS  | 2.0  |
| 9   | CI    | 63   | ILE  | 2.0  |
| 11  | AK    | 11   | LYS  | 2.0  |
| 43  | DU    | 109  | LEU  | 2.0  |
| 58  | D9    | 33   | LYS  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | AB    | 209 | ARG  | 2.0  |
| 34  | DH    | 31  | GLY  | 2.0  |
| 1   | AA    | 96  | U    | 2.0  |
| 7   | AG    | 80  | VAL  | 2.0  |
| 29  | BC    | 100 | ILE  | 2.0  |
| 34  | DH    | 89  | ILE  | 2.0  |
| 52  | B3    | 44  | ARG  | 2.0  |
| 4   | CD    | 156 | GLU  | 2.0  |
| 29  | BC    | 85  | GLU  | 2.0  |
| 24  | AX    | 61  | C    | 2.0  |
| 24  | AX    | 62  | C    | 2.0  |
| 43  | DU    | 85  | LYS  | 2.0  |
| 13  | AM    | 87  | TYR  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 26  | DPP  | CZ    | 2   | 6/7   | 0.83 | 0.15 | -    | 94,96,97,97                | 0     |
| 26  | UAL  | AZ    | 5   | 9/10  | 0.81 | 0.20 | -    | 81,82,83,84                | 0     |
| 26  | DPP  | AZ    | 2   | 6/7   | 0.93 | 0.16 | -    | 79,82,82,84                | 0     |
| 26  | UAL  | CZ    | 5   | 9/10  | 0.78 | 0.27 | -    | 97,99,99,99                | 0     |
| 26  | 5OH  | AZ    | 6   | 12/13 | 0.87 | 0.18 | -    | 84,89,92,94                | 0     |
| 26  | KBE  | AZ    | 1   | 9/10  | 0.85 | 0.34 | -    | 78,79,82,82                | 0     |
| 26  | 5OH  | CZ    | 6   | 12/13 | 0.89 | 0.27 | -    | 99,101,102,102             | 0     |
| 26  | KBE  | CZ    | 1   | 9/10  | 0.79 | 0.36 | -    | 89,91,93,94                | 0     |

## 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 59  | MG   | BA    | 3056 | 1/1   | 0.92 | 0.66 | 34.54 | 59,59,59,59                | 0     |
| 59  | MG   | BA    | 3134 | 1/1   | 0.70 | 0.57 | 31.90 | 39,39,39,39                | 0     |
| 59  | MG   | DA    | 3082 | 1/1   | 0.91 | 0.47 | 24.31 | 37,37,37,37                | 0     |
| 59  | MG   | CA    | 1615 | 1/1   | 0.92 | 0.62 | 22.75 | 51,51,51,51                | 0     |
| 59  | MG   | AA    | 1603 | 1/1   | 0.89 | 0.51 | 22.09 | 58,58,58,58                | 0     |
| 59  | MG   | BA    | 3295 | 1/1   | 0.89 | 0.42 | 21.25 | 47,47,47,47                | 0     |
| 59  | MG   | BA    | 3188 | 1/1   | 0.97 | 0.42 | 20.02 | 22,22,22,22                | 0     |
| 59  | MG   | DA    | 3177 | 1/1   | 0.98 | 0.42 | 18.86 | 29,29,29,29                | 0     |
| 59  | MG   | DA    | 3152 | 1/1   | 0.82 | 0.40 | 17.18 | 54,54,54,54                | 0     |
| 59  | MG   | BA    | 3088 | 1/1   | 0.97 | 0.34 | 17.00 | 22,22,22,22                | 0     |
| 59  | MG   | CA    | 1606 | 1/1   | 0.96 | 0.66 | 16.88 | 52,52,52,52                | 0     |
| 59  | MG   | DE    | 302  | 1/1   | 0.93 | 0.65 | 14.66 | 65,65,65,65                | 0     |
| 59  | MG   | DA    | 3249 | 1/1   | 0.95 | 0.40 | 14.55 | 54,54,54,54                | 0     |
| 59  | MG   | DA    | 3097 | 1/1   | 0.88 | 0.37 | 14.14 | 65,65,65,65                | 0     |
| 59  | MG   | AX    | 105  | 1/1   | 0.69 | 0.39 | 13.94 | 82,82,82,82                | 0     |
| 59  | MG   | BA    | 3216 | 1/1   | 0.85 | 0.41 | 13.82 | 42,42,42,42                | 0     |
| 59  | MG   | DA    | 3164 | 1/1   | 0.90 | 0.38 | 13.81 | 51,51,51,51                | 0     |
| 59  | MG   | CA    | 1620 | 1/1   | 0.95 | 0.40 | 12.33 | 40,40,40,40                | 0     |
| 59  | MG   | BA    | 3154 | 1/1   | 0.79 | 0.30 | 11.68 | 44,44,44,44                | 0     |
| 59  | MG   | DA    | 3035 | 1/1   | 0.92 | 0.64 | 11.62 | 63,63,63,63                | 0     |
| 59  | MG   | AA    | 1619 | 1/1   | 0.94 | 0.55 | 11.33 | 47,47,47,47                | 0     |
| 59  | MG   | BA    | 3194 | 1/1   | 0.97 | 0.31 | 11.27 | 33,33,33,33                | 0     |
| 59  | MG   | DA    | 3257 | 1/1   | 0.90 | 0.49 | 10.74 | 40,40,40,40                | 0     |
| 59  | MG   | BA    | 3337 | 1/1   | 0.83 | 0.36 | 10.51 | 61,61,61,61                | 0     |
| 59  | MG   | DA    | 3007 | 1/1   | 0.82 | 0.32 | 10.50 | 42,42,42,42                | 0     |
| 59  | MG   | BA    | 3213 | 1/1   | 0.95 | 0.54 | 10.30 | 54,54,54,54                | 0     |
| 59  | MG   | BA    | 3161 | 1/1   | 0.99 | 0.44 | 10.01 | 16,16,16,16                | 0     |
| 59  | MG   | BA    | 3128 | 1/1   | 0.92 | 0.43 | 9.99  | 34,34,34,34                | 0     |
| 59  | MG   | AA    | 1640 | 1/1   | 0.90 | 0.36 | 9.31  | 37,37,37,37                | 0     |
| 59  | MG   | BA    | 3010 | 1/1   | 0.80 | 0.32 | 9.12  | 29,29,29,29                | 0     |
| 59  | MG   | BA    | 3251 | 1/1   | 0.96 | 0.27 | 8.97  | 34,34,34,34                | 0     |
| 59  | MG   | DA    | 3216 | 1/1   | 0.95 | 0.30 | 8.79  | 35,35,35,35                | 0     |
| 59  | MG   | DA    | 3061 | 1/1   | 0.89 | 0.31 | 8.76  | 28,28,28,28                | 0     |
| 59  | MG   | BA    | 3341 | 1/1   | 0.91 | 0.28 | 8.63  | 86,86,86,86                | 0     |
| 59  | MG   | DA    | 3108 | 1/1   | 0.68 | 0.34 | 8.41  | 51,51,51,51                | 0     |
| 59  | MG   | AA    | 1677 | 1/1   | 0.97 | 0.38 | 8.28  | 75,75,75,75                | 0     |
| 59  | MG   | BA    | 3023 | 1/1   | 0.98 | 0.25 | 8.11  | 23,23,23,23                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | DD    | 301  | 1/1   | 0.13 | 0.57 | 7.99 | 110,110,110,110             | 0     |
| 59  | MG   | DA    | 3005 | 1/1   | 0.86 | 0.25 | 7.71 | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3147 | 1/1   | 0.98 | 0.40 | 7.29 | 44,44,44,44                 | 0     |
| 59  | MG   | CA    | 1639 | 1/1   | 0.89 | 0.31 | 7.05 | 74,74,74,74                 | 0     |
| 59  | MG   | BA    | 3115 | 1/1   | 0.97 | 0.27 | 6.87 | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3018 | 1/1   | 0.98 | 0.25 | 6.84 | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3003 | 1/1   | 0.93 | 0.22 | 6.64 | 36,36,36,36                 | 0     |
| 59  | MG   | CA    | 1610 | 1/1   | 0.96 | 0.34 | 6.53 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3192 | 1/1   | 0.98 | 0.25 | 6.44 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3081 | 1/1   | 0.98 | 0.33 | 6.30 | 6,6,6,6                     | 0     |
| 59  | MG   | AA    | 1637 | 1/1   | 0.85 | 0.21 | 6.26 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3183 | 1/1   | 0.92 | 0.23 | 5.95 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3079 | 1/1   | 0.92 | 0.28 | 5.89 | 16,16,16,16                 | 0     |
| 59  | MG   | AA    | 1665 | 1/1   | 0.81 | 0.27 | 5.83 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3193 | 1/1   | 0.95 | 0.36 | 5.82 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3095 | 1/1   | 0.95 | 0.25 | 5.64 | 30,30,30,30                 | 0     |
| 59  | MG   | DA    | 3015 | 1/1   | 0.97 | 0.42 | 5.54 | 37,37,37,37                 | 0     |
| 59  | MG   | BU    | 201  | 1/1   | 0.94 | 0.27 | 5.18 | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3345 | 1/1   | 0.96 | 0.24 | 4.96 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3243 | 1/1   | 0.92 | 0.38 | 4.90 | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3066 | 1/1   | 0.97 | 0.29 | 4.80 | 20,20,20,20                 | 0     |
| 59  | MG   | DA    | 3112 | 1/1   | 0.80 | 0.22 | 4.73 | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3050 | 1/1   | 0.97 | 0.28 | 4.57 | 4,4,4,4                     | 0     |
| 59  | MG   | BA    | 3223 | 1/1   | 0.94 | 0.24 | 4.47 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3012 | 1/1   | 0.98 | 0.29 | 4.23 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3039 | 1/1   | 0.94 | 0.32 | 4.13 | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1616 | 1/1   | 0.96 | 0.24 | 4.07 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3077 | 1/1   | 0.73 | 0.32 | 4.03 | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3047 | 1/1   | 0.96 | 0.22 | 3.97 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3189 | 1/1   | 0.94 | 0.31 | 3.96 | 18,18,18,18                 | 0     |
| 59  | MG   | DA    | 3130 | 1/1   | 0.99 | 0.31 | 3.94 | 27,27,27,27                 | 0     |
| 59  | MG   | CA    | 1642 | 1/1   | 0.91 | 0.24 | 3.81 | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1622 | 1/1   | 0.95 | 0.29 | 3.72 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3106 | 1/1   | 0.95 | 0.30 | 3.62 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3021 | 1/1   | 0.98 | 0.25 | 3.58 | 3,3,3,3                     | 0     |
| 59  | MG   | BA    | 3336 | 1/1   | 0.94 | 0.31 | 3.57 | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3241 | 1/1   | 0.94 | 0.29 | 3.47 | 42,42,42,42                 | 0     |
| 59  | MG   | CA    | 1633 | 1/1   | 0.98 | 0.22 | 3.37 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3002 | 1/1   | 0.94 | 0.24 | 3.34 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3099 | 1/1   | 0.79 | 0.30 | 3.28 | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3043 | 1/1   | 0.85 | 0.33 | 2.99 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3381 | 1/1   | 0.90 | 0.16 | 2.98 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3199 | 1/1   | 0.95 | 0.25 | 2.90 | 54,54,54,54                 | 0     |
| 59  | MG   | CA    | 1629 | 1/1   | 0.95 | 0.29 | 2.70 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3024 | 1/1   | 0.95 | 0.18 | 2.61 | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3091 | 1/1   | 0.94 | 0.23 | 2.43 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3120 | 1/1   | 0.88 | 0.29 | 2.42 | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1663 | 1/1   | 0.98 | 0.20 | 2.40 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3014 | 1/1   | 0.96 | 0.24 | 2.40 | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1697 | 1/1   | 0.95 | 0.34 | 2.34 | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3151 | 1/1   | 0.95 | 0.29 | 2.30 | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3010 | 1/1   | 0.98 | 0.26 | 2.20 | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3020 | 1/1   | 0.94 | 0.23 | 2.09 | 22,22,22,22                 | 0     |
| 59  | MG   | AA    | 1614 | 1/1   | 0.95 | 0.20 | 1.82 | 45,45,45,45                 | 0     |
| 59  | MG   | AA    | 1656 | 1/1   | 0.89 | 0.21 | 1.68 | 42,42,42,42                 | 0     |
| 59  | MG   | CA    | 1656 | 1/1   | 0.96 | 0.22 | 1.64 | 51,51,51,51                 | 0     |
| 59  | MG   | D5    | 102  | 1/1   | 0.95 | 0.22 | 1.53 | 91,91,91,91                 | 0     |
| 59  | MG   | BA    | 3053 | 1/1   | 0.90 | 0.22 | 1.52 | 11,11,11,11                 | 0     |
| 59  | MG   | AA    | 1717 | 1/1   | 0.84 | 0.18 | 1.47 | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3192 | 1/1   | 0.90 | 0.22 | 1.45 | 39,39,39,39                 | 0     |
| 59  | MG   | DA    | 3205 | 1/1   | 0.99 | 0.25 | 1.44 | 27,27,27,27                 | 0     |
| 59  | MG   | DA    | 3012 | 1/1   | 0.96 | 0.25 | 1.42 | 33,33,33,33                 | 0     |
| 59  | MG   | CA    | 1638 | 1/1   | 0.85 | 0.20 | 1.40 | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1690 | 1/1   | 0.98 | 0.21 | 1.26 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3116 | 1/1   | 0.84 | 0.21 | 1.25 | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3153 | 1/1   | 0.93 | 0.18 | 1.23 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3001 | 1/1   | 0.96 | 0.18 | 1.11 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3142 | 1/1   | 0.95 | 0.26 | 1.11 | 18,18,18,18                 | 0     |
| 59  | MG   | DA    | 3081 | 1/1   | 0.96 | 0.20 | 1.06 | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3096 | 1/1   | 0.98 | 0.19 | 0.93 | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1673 | 1/1   | 0.97 | 0.20 | 0.91 | 35,35,35,35                 | 0     |
| 59  | MG   | B0    | 101  | 1/1   | 0.87 | 0.25 | 0.91 | 58,58,58,58                 | 0     |
| 59  | MG   | DA    | 3106 | 1/1   | 0.97 | 0.21 | 0.88 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1641 | 1/1   | 0.78 | 0.20 | 0.87 | 62,62,62,62                 | 0     |
| 59  | MG   | CA    | 1669 | 1/1   | 0.89 | 0.17 | 0.87 | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3048 | 1/1   | 0.98 | 0.18 | 0.86 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3257 | 1/1   | 0.90 | 0.21 | 0.77 | 21,21,21,21                 | 0     |
| 59  | MG   | DA    | 3206 | 1/1   | 0.99 | 0.26 | 0.71 | 27,27,27,27                 | 0     |
| 59  | MG   | DA    | 3090 | 1/1   | 0.98 | 0.19 | 0.54 | 24,24,24,24                 | 0     |
| 59  | MG   | DA    | 3131 | 1/1   | 0.96 | 0.17 | 0.52 | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3167 | 1/1   | 0.89 | 0.20 | 0.52 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3037 | 1/1   | 0.96 | 0.17 | 0.46 | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3334 | 1/1   | 0.89 | 0.18 | 0.45 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 59  | MG   | BA    | 3087 | 1/1   | 0.83 | 0.21 | 0.39  | 39,39,39,39                | 0     |
| 60  | ZN   | D4    | 101  | 1/1   | 0.94 | 0.17 | 0.35  | 147,147,147,147            | 0     |
| 59  | MG   | CX    | 103  | 1/1   | 0.96 | 0.21 | 0.30  | 50,50,50,50                | 0     |
| 59  | MG   | BA    | 3217 | 1/1   | 0.97 | 0.17 | 0.03  | 11,11,11,11                | 0     |
| 59  | MG   | DA    | 3091 | 1/1   | 0.92 | 0.18 | 0.02  | 67,67,67,67                | 0     |
| 59  | MG   | DA    | 3182 | 1/1   | 0.98 | 0.16 | -0.06 | 33,33,33,33                | 0     |
| 59  | MG   | DA    | 3098 | 1/1   | 0.86 | 0.17 | -0.09 | 37,37,37,37                | 0     |
| 60  | ZN   | CD    | 301  | 1/1   | 0.97 | 0.25 | -0.10 | 61,61,61,61                | 0     |
| 59  | MG   | BF    | 302  | 1/1   | 0.89 | 0.18 | -0.16 | 26,26,26,26                | 0     |
| 59  | MG   | DA    | 3017 | 1/1   | 0.92 | 0.22 | -0.17 | 16,16,16,16                | 0     |
| 59  | MG   | AA    | 1657 | 1/1   | 0.97 | 0.16 | -0.41 | 53,53,53,53                | 0     |
| 59  | MG   | AA    | 1611 | 1/1   | 0.95 | 0.16 | -0.48 | 52,52,52,52                | 0     |
| 59  | MG   | BA    | 3137 | 1/1   | 0.95 | 0.17 | -0.54 | 34,34,34,34                | 0     |
| 59  | MG   | BA    | 3123 | 1/1   | 0.95 | 0.17 | -0.55 | 45,45,45,45                | 0     |
| 59  | MG   | BA    | 3203 | 1/1   | 0.97 | 0.16 | -0.55 | 38,38,38,38                | 0     |
| 59  | MG   | AA    | 1602 | 1/1   | 0.98 | 0.16 | -0.57 | 44,44,44,44                | 0     |
| 60  | ZN   | AD    | 302  | 1/1   | 0.95 | 0.24 | -0.63 | 67,67,67,67                | 0     |
| 59  | MG   | CA    | 1658 | 1/1   | 0.97 | 0.14 | -0.67 | 40,40,40,40                | 0     |
| 59  | MG   | CA    | 1678 | 1/1   | 0.97 | 0.17 | -0.69 | 45,45,45,45                | 0     |
| 59  | MG   | BY    | 201  | 1/1   | 0.99 | 0.16 | -0.71 | 32,32,32,32                | 0     |
| 59  | MG   | BA    | 3124 | 1/1   | 0.98 | 0.15 | -0.72 | 27,27,27,27                | 0     |
| 59  | MG   | BA    | 3090 | 1/1   | 0.97 | 0.14 | -0.76 | 32,32,32,32                | 0     |
| 59  | MG   | CA    | 1614 | 1/1   | 0.94 | 0.16 | -0.78 | 49,49,49,49                | 0     |
| 59  | MG   | BA    | 3083 | 1/1   | 0.95 | 0.17 | -0.78 | 6,6,6,6                    | 0     |
| 59  | MG   | BA    | 3288 | 1/1   | 0.90 | 0.16 | -0.80 | 33,33,33,33                | 0     |
| 59  | MG   | AX    | 103  | 1/1   | 0.94 | 0.14 | -0.83 | 32,32,32,32                | 0     |
| 59  | MG   | BA    | 3121 | 1/1   | 0.96 | 0.16 | -0.90 | 38,38,38,38                | 0     |
| 59  | MG   | BA    | 3238 | 1/1   | 0.95 | 0.14 | -0.91 | 26,26,26,26                | 0     |
| 59  | MG   | BA    | 3107 | 1/1   | 0.97 | 0.16 | -0.93 | 13,13,13,13                | 0     |
| 59  | MG   | BA    | 3387 | 1/1   | 0.99 | 0.13 | -0.95 | 46,46,46,46                | 0     |
| 59  | MG   | DA    | 3155 | 1/1   | 0.94 | 0.17 | -1.04 | 56,56,56,56                | 0     |
| 59  | MG   | AA    | 1669 | 1/1   | 0.96 | 0.15 | -1.04 | 36,36,36,36                | 0     |
| 59  | MG   | BA    | 3022 | 1/1   | 0.96 | 0.16 | -1.04 | 12,12,12,12                | 0     |
| 59  | MG   | AA    | 1720 | 1/1   | 0.96 | 0.16 | -1.05 | 52,52,52,52                | 0     |
| 59  | MG   | DA    | 3128 | 1/1   | 0.93 | 0.14 | -1.06 | 26,26,26,26                | 0     |
| 59  | MG   | BA    | 3212 | 1/1   | 0.99 | 0.14 | -1.08 | 25,25,25,25                | 0     |
| 59  | MG   | BA    | 3279 | 1/1   | 0.98 | 0.16 | -1.09 | 62,62,62,62                | 0     |
| 59  | MG   | BA    | 3093 | 1/1   | 0.94 | 0.15 | -1.11 | 10,10,10,10                | 0     |
| 59  | MG   | DA    | 3150 | 1/1   | 0.96 | 0.18 | -1.12 | 43,43,43,43                | 0     |
| 59  | MG   | CQ    | 201  | 1/1   | 0.82 | 0.12 | -1.14 | 94,94,94,94                | 0     |
| 59  | MG   | BA    | 3150 | 1/1   | 0.95 | 0.14 | -1.17 | 33,33,33,33                | 0     |
| 59  | MG   | DA    | 3101 | 1/1   | 0.92 | 0.09 | -1.17 | 28,28,28,28                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 59  | MG   | DA    | 3190 | 1/1   | 0.76 | 0.14 | -1.22 | 33,33,33,33                 | 0     |
| 59  | MG   | DE    | 303  | 1/1   | 0.89 | 0.11 | -1.24 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3009 | 1/1   | 0.93 | 0.15 | -1.24 | 20,20,20,20                 | 0     |
| 59  | MG   | AA    | 1661 | 1/1   | 0.94 | 0.14 | -1.26 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3144 | 1/1   | 0.92 | 0.14 | -1.32 | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3157 | 1/1   | 0.93 | 0.13 | -1.36 | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3202 | 1/1   | 0.95 | 0.11 | -1.42 | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1681 | 1/1   | 0.96 | 0.08 | -1.46 | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1684 | 1/1   | 0.89 | 0.08 | -1.48 | 42,42,42,42                 | 0     |
| 60  | ZN   | B5    | 102  | 1/1   | 0.92 | 0.07 | -1.49 | 75,75,75,75                 | 0     |
| 59  | MG   | DA    | 3246 | 1/1   | 0.99 | 0.14 | -1.50 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3258 | 1/1   | 0.96 | 0.13 | -1.50 | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3306 | 1/1   | 0.93 | 0.15 | -1.52 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3202 | 1/1   | 0.95 | 0.12 | -1.54 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3065 | 1/1   | 0.98 | 0.10 | -1.62 | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3073 | 1/1   | 0.93 | 0.16 | -1.63 | 10,10,10,10                 | 0     |
| 60  | ZN   | B9    | 101  | 1/1   | 0.98 | 0.06 | -1.65 | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3181 | 1/1   | 0.93 | 0.10 | -1.69 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3052 | 1/1   | 0.90 | 0.15 | -1.70 | 30,30,30,30                 | 0     |
| 59  | MG   | DA    | 3070 | 1/1   | 0.97 | 0.14 | -1.71 | 10,10,10,10                 | 0     |
| 59  | MG   | CA    | 1660 | 1/1   | 0.95 | 0.11 | -1.73 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3385 | 1/1   | 0.96 | 0.11 | -1.74 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3168 | 1/1   | 0.96 | 0.15 | -1.74 | 37,37,37,37                 | 0     |
| 59  | MG   | AA    | 1629 | 1/1   | 0.94 | 0.14 | -1.76 | 78,78,78,78                 | 0     |
| 59  | MG   | CA    | 1640 | 1/1   | 0.96 | 0.10 | -1.80 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3044 | 1/1   | 0.95 | 0.13 | -1.85 | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3137 | 1/1   | 0.85 | 0.12 | -1.85 | 28,28,28,28                 | 0     |
| 59  | MG   | DA    | 3063 | 1/1   | 0.97 | 0.15 | -1.87 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3062 | 1/1   | 0.99 | 0.14 | -1.95 | 14,14,14,14                 | 0     |
| 59  | MG   | BF    | 301  | 1/1   | 0.92 | 0.15 | -1.97 | 37,37,37,37                 | 0     |
| 60  | ZN   | B4    | 101  | 1/1   | 0.92 | 0.06 | -2.02 | 117,117,117,117             | 0     |
| 59  | MG   | DA    | 3001 | 1/1   | 0.98 | 0.09 | -2.02 | 25,25,25,25                 | 0     |
| 59  | MG   | CA    | 1604 | 1/1   | 0.96 | 0.11 | -2.03 | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3079 | 1/1   | 0.92 | 0.15 | -2.03 | 23,23,23,23                 | 0     |
| 59  | MG   | AA    | 1687 | 1/1   | 0.95 | 0.06 | -2.06 | 27,27,27,27                 | 0     |
| 59  | MG   | DF    | 301  | 1/1   | 0.94 | 0.09 | -2.07 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3107 | 1/1   | 0.96 | 0.11 | -2.08 | 32,32,32,32                 | 0     |
| 59  | MG   | CA    | 1624 | 1/1   | 0.97 | 0.15 | -2.09 | 24,24,24,24                 | 0     |
| 59  | MG   | DA    | 3124 | 1/1   | 0.94 | 0.05 | -2.20 | 43,43,43,43                 | 0     |
| 59  | MG   | BQ    | 201  | 1/1   | 0.95 | 0.14 | -2.28 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3011 | 1/1   | 0.96 | 0.13 | -2.33 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3075 | 1/1   | 0.99 | 0.13 | -2.35 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60  | ZN   | D9    | 101  | 1/1   | 0.95 | 0.02 | -2.36 | 109,109,109,109             | 0     |
| 59  | MG   | BA    | 3233 | 1/1   | 0.92 | 0.13 | -2.41 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3049 | 1/1   | 0.91 | 0.11 | -2.42 | 12,12,12,12                 | 0     |
| 59  | MG   | BA    | 3218 | 1/1   | 0.95 | 0.12 | -2.45 | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3112 | 1/1   | 0.85 | 0.13 | -2.46 | 52,52,52,52                 | 0     |
| 60  | ZN   | D5    | 103  | 1/1   | 0.88 | 0.05 | -2.47 | 92,92,92,92                 | 0     |
| 59  | MG   | DA    | 3054 | 1/1   | 0.96 | 0.11 | -2.48 | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3165 | 1/1   | 0.95 | 0.07 | -2.51 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3169 | 1/1   | 0.98 | 0.12 | -2.60 | 51,51,51,51                 | 0     |
| 59  | MG   | DA    | 3110 | 1/1   | 0.96 | 0.09 | -2.97 | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3082 | 1/1   | 0.95 | 0.12 | -2.99 | 15,15,15,15                 | 0     |
| 59  | MG   | AA    | 1664 | 1/1   | 0.96 | 0.10 | -3.00 | 20,20,20,20                 | 0     |
| 59  | MG   | DA    | 3262 | 1/1   | 0.92 | 0.08 | -3.07 | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1683 | 1/1   | 0.96 | 0.10 | -3.11 | 31,31,31,31                 | 0     |
| 59  | MG   | AA    | 1709 | 1/1   | 0.99 | 0.11 | -3.12 | 44,44,44,44                 | 0     |
| 59  | MG   | AA    | 1633 | 1/1   | 0.92 | 0.08 | -3.15 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3103 | 1/1   | 0.92 | 0.07 | -3.39 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3237 | 1/1   | 0.95 | 0.09 | -3.49 | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3155 | 1/1   | 0.98 | 0.08 | -3.50 | 9,9,9,9                     | 0     |
| 59  | MG   | BA    | 3054 | 1/1   | 0.93 | 0.12 | -3.55 | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3057 | 1/1   | 0.91 | 0.15 | -3.67 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3005 | 1/1   | 0.97 | 0.08 | -3.68 | 17,17,17,17                 | 0     |
| 59  | MG   | AA    | 1616 | 1/1   | 0.98 | 0.08 | -3.74 | 16,16,16,16                 | 0     |
| 59  | MG   | AA    | 1631 | 1/1   | 0.99 | 0.10 | -3.77 | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3173 | 1/1   | 0.94 | 0.11 | -3.82 | 17,17,17,17                 | 0     |
| 59  | MG   | DA    | 3045 | 1/1   | 0.90 | 0.13 | -3.96 | 41,41,41,41                 | 0     |
| 59  | MG   | DA    | 3139 | 1/1   | 0.96 | 0.08 | -3.97 | 18,18,18,18                 | 0     |
| 59  | MG   | CA    | 1637 | 1/1   | 0.95 | 0.07 | -3.97 | 29,29,29,29                 | 0     |
| 59  | MG   | DA    | 3057 | 1/1   | 0.92 | 0.11 | -4.05 | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3255 | 1/1   | 0.93 | 0.12 | -4.09 | 22,22,22,22                 | 0     |
| 59  | MG   | AA    | 1679 | 1/1   | 0.99 | 0.04 | -4.09 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3101 | 1/1   | 0.97 | 0.11 | -4.27 | 25,25,25,25                 | 0     |
| 59  | MG   | DA    | 3116 | 1/1   | 0.95 | 0.13 | -4.36 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3301 | 1/1   | 0.94 | 0.11 | -4.47 | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3130 | 1/1   | 0.97 | 0.08 | -4.60 | 13,13,13,13                 | 0     |
| 59  | MG   | CA    | 1685 | 1/1   | 0.97 | 0.08 | -4.89 | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3040 | 1/1   | 0.98 | 0.05 | -5.02 | 9,9,9,9                     | 0     |
| 59  | MG   | BA    | 3368 | 1/1   | 0.97 | 0.10 | -5.03 | 24,24,24,24                 | 0     |
| 59  | MG   | BA    | 3077 | 1/1   | 0.98 | 0.07 | -5.25 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3361 | 1/1   | 0.95 | 0.11 | -5.47 | 25,25,25,25                 | 0     |
| 59  | MG   | CA    | 1634 | 1/1   | 0.98 | 0.04 | -5.67 | 17,17,17,17                 | 0     |
| 59  | MG   | DA    | 3008 | 1/1   | 0.99 | 0.05 | -5.78 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 59  | MG   | BA    | 3204 | 1/1   | 0.96 | 0.10 | -5.89 | 2,2,2,2                     | 0     |
| 59  | MG   | DA    | 3023 | 1/1   | 0.99 | 0.05 | -5.96 | 33,33,33,33                 | 0     |
| 59  | MG   | DA    | 3256 | 1/1   | 0.94 | 0.12 | -6.06 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3344 | 1/1   | 0.89 | 0.10 | -6.75 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3114 | 1/1   | 0.98 | 0.08 | -8.26 | 42,42,42,42                 | 0     |
| 59  | MG   | D6    | 101  | 1/1   | 0.95 | 0.30 | -     | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3041 | 1/1   | 0.97 | 0.29 | -     | 7,7,7,7                     | 0     |
| 59  | MG   | BA    | 3360 | 1/1   | 0.82 | 0.40 | -     | 68,68,68,68                 | 0     |
| 59  | MG   | CA    | 1631 | 1/1   | 0.87 | 0.47 | -     | 45,45,45,45                 | 0     |
| 59  | MG   | AA    | 1731 | 1/1   | 0.91 | 0.17 | -     | 22,22,22,22                 | 0     |
| 59  | MG   | CA    | 1652 | 1/1   | 0.85 | 0.37 | -     | 86,86,86,86                 | 0     |
| 59  | MG   | DA    | 3184 | 1/1   | 0.92 | 0.11 | -     | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1663 | 1/1   | 0.94 | 0.44 | -     | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3236 | 1/1   | 0.87 | 1.01 | -     | 91,91,91,91                 | 0     |
| 59  | MG   | CA    | 1655 | 1/1   | 0.99 | 0.29 | -     | 41,41,41,41                 | 0     |
| 59  | MG   | DA    | 3250 | 1/1   | 0.82 | 0.41 | -     | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3158 | 1/1   | 0.95 | 0.33 | -     | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3355 | 1/1   | 0.97 | 0.17 | -     | 33,33,33,33                 | 0     |
| 59  | MG   | DA    | 3069 | 1/1   | 0.45 | 0.83 | -     | 78,78,78,78                 | 0     |
| 59  | MG   | AA    | 1644 | 1/1   | 0.95 | 0.24 | -     | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3266 | 1/1   | 0.98 | 0.38 | -     | 72,72,72,72                 | 0     |
| 59  | MG   | CA    | 1686 | 1/1   | 0.77 | 0.30 | -     | 64,64,64,64                 | 0     |
| 59  | MG   | DD    | 303  | 1/1   | 0.82 | 0.51 | -     | 95,95,95,95                 | 0     |
| 59  | MG   | AA    | 1713 | 1/1   | 0.98 | 0.16 | -     | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3156 | 1/1   | 0.85 | 0.29 | -     | 25,25,25,25                 | 0     |
| 59  | MG   | DA    | 3209 | 1/1   | 0.91 | 0.44 | -     | 69,69,69,69                 | 0     |
| 59  | MG   | CA    | 1630 | 1/1   | 0.63 | 0.37 | -     | 55,55,55,55                 | 0     |
| 59  | MG   | AA    | 1685 | 1/1   | 0.91 | 0.55 | -     | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3083 | 1/1   | 0.96 | 0.31 | -     | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3133 | 1/1   | 0.89 | 0.17 | -     | 20,20,20,20                 | 0     |
| 59  | MG   | CX    | 101  | 1/1   | 0.90 | 0.12 | -     | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3196 | 1/1   | 0.89 | 0.40 | -     | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3186 | 1/1   | 0.96 | 0.21 | -     | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3296 | 1/1   | 0.72 | 0.27 | -     | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3215 | 1/1   | 0.97 | 0.15 | -     | 12,12,12,12                 | 0     |
| 59  | MG   | DA    | 3233 | 1/1   | 0.98 | 0.35 | -     | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1678 | 1/1   | 0.85 | 0.21 | -     | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3250 | 1/1   | 0.98 | 0.13 | -     | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3384 | 1/1   | 0.94 | 0.10 | -     | 39,39,39,39                 | 0     |
| 59  | MG   | AA    | 1627 | 1/1   | 0.76 | 0.40 | -     | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3221 | 1/1   | 0.96 | 0.24 | -     | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3206 | 1/1   | 0.95 | 0.17 | -     | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3092 | 1/1   | 0.98 | 0.36 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | CA    | 1687 | 1/1   | 0.92 | 0.14 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | CA    | 1623 | 1/1   | 0.76 | 0.21 | -    | 91,91,91,91                 | 0     |
| 59  | MG   | BA    | 3129 | 1/1   | 0.99 | 0.12 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1703 | 1/1   | 0.94 | 0.08 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | CA    | 1673 | 1/1   | 0.96 | 0.32 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3274 | 1/1   | 0.90 | 0.15 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3132 | 1/1   | 0.81 | 0.22 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | CA    | 1677 | 1/1   | 0.85 | 0.15 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3386 | 1/1   | 0.88 | 0.18 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | AA    | 1649 | 1/1   | 0.92 | 0.36 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | CA    | 1646 | 1/1   | 0.96 | 0.32 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3015 | 1/1   | 0.98 | 0.38 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3109 | 1/1   | 0.93 | 0.14 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1676 | 1/1   | 0.68 | 0.19 | -    | 77,77,77,77                 | 0     |
| 59  | MG   | AA    | 1721 | 1/1   | 0.93 | 0.14 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3224 | 1/1   | 0.74 | 0.28 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3017 | 1/1   | 0.98 | 0.19 | -    | 14,14,14,14                 | 0     |
| 59  | MG   | DA    | 3232 | 1/1   | 0.92 | 0.29 | -    | 80,80,80,80                 | 0     |
| 59  | MG   | DA    | 3261 | 1/1   | 0.91 | 0.32 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | AW    | 105  | 1/1   | 0.87 | 0.21 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | DA    | 3033 | 1/1   | 0.97 | 0.12 | -    | 10,10,10,10                 | 0     |
| 59  | MG   | DA    | 3208 | 1/1   | 0.94 | 0.40 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BN    | 201  | 1/1   | 0.83 | 0.35 | -    | 67,67,67,67                 | 0     |
| 59  | MG   | AW    | 102  | 1/1   | 0.81 | 0.12 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3209 | 1/1   | 0.95 | 0.11 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1726 | 1/1   | 0.95 | 0.29 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3258 | 1/1   | 0.97 | 0.19 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | DA    | 3230 | 1/1   | 0.93 | 0.51 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | AT    | 202  | 1/1   | 0.90 | 0.42 | -    | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3317 | 1/1   | 0.79 | 0.41 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1674 | 1/1   | 0.95 | 0.05 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | CA    | 1607 | 1/1   | 0.88 | 0.41 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3346 | 1/1   | 0.79 | 0.33 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1630 | 1/1   | 0.96 | 0.07 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | DZ    | 301  | 1/1   | 0.90 | 0.21 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3316 | 1/1   | 0.88 | 0.43 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3359 | 1/1   | 0.91 | 0.32 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BR    | 201  | 1/1   | 0.84 | 0.44 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3269 | 1/1   | 0.77 | 0.95 | -    | 83,83,83,83                 | 0     |
| 59  | MG   | BA    | 3205 | 1/1   | 0.85 | 0.28 | -    | 86,86,86,86                 | 0     |
| 59  | MG   | CA    | 1625 | 1/1   | 0.90 | 0.55 | -    | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1716 | 1/1   | 0.92 | 0.23 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | AA    | 1634 | 1/1   | 0.83 | 0.12 | -    | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3100 | 1/1   | 0.97 | 0.21 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3105 | 1/1   | 0.97 | 0.22 | -    | 14,14,14,14                 | 0     |
| 59  | MG   | AA    | 1680 | 1/1   | 0.95 | 0.41 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3201 | 1/1   | 0.95 | 0.17 | -    | 111,111,111,111             | 0     |
| 59  | MG   | BE    | 301  | 1/1   | 0.97 | 0.23 | -    | 12,12,12,12                 | 0     |
| 59  | MG   | BA    | 3063 | 1/1   | 0.99 | 0.23 | -    | 19,19,19,19                 | 0     |
| 59  | MG   | CA    | 1674 | 1/1   | 0.92 | 0.33 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3260 | 1/1   | 0.88 | 0.17 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1627 | 1/1   | 0.94 | 0.15 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3167 | 1/1   | 0.90 | 0.15 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | AX    | 101  | 1/1   | 0.90 | 0.41 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3185 | 1/1   | 0.97 | 0.08 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3267 | 1/1   | 0.96 | 0.12 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3311 | 1/1   | 0.95 | 0.86 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | DB    | 201  | 1/1   | 0.85 | 0.15 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | AY    | 102  | 1/1   | 0.81 | 0.52 | -    | 96,96,96,96                 | 0     |
| 59  | MG   | DA    | 3056 | 1/1   | 0.98 | 0.21 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3030 | 1/1   | 0.96 | 0.13 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | AA    | 1732 | 1/1   | 0.92 | 0.16 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1612 | 1/1   | 0.98 | 0.04 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1714 | 1/1   | 0.87 | 0.37 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | AA    | 1646 | 1/1   | 0.80 | 0.30 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3178 | 1/1   | 0.97 | 0.37 | -    | 11,11,11,11                 | 0     |
| 59  | MG   | BA    | 3353 | 1/1   | 0.97 | 0.38 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | CA    | 1684 | 1/1   | 0.95 | 0.51 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1659 | 1/1   | 0.87 | 0.10 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3191 | 1/1   | 0.88 | 0.19 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3200 | 1/1   | 0.88 | 0.31 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3214 | 1/1   | 0.88 | 0.33 | -    | 87,87,87,87                 | 0     |
| 59  | MG   | BZ    | 301  | 1/1   | 0.84 | 0.15 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1698 | 1/1   | 0.91 | 0.19 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1626 | 1/1   | 0.96 | 0.11 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3147 | 1/1   | 0.86 | 0.25 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3035 | 1/1   | 0.95 | 0.17 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | AA    | 1727 | 1/1   | 0.72 | 0.54 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | AW    | 104  | 1/1   | 0.87 | 0.14 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3135 | 1/1   | 0.93 | 0.26 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3025 | 1/1   | 0.97 | 0.17 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3245 | 1/1   | 0.89 | 0.67 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | AW    | 103  | 1/1   | 0.82 | 0.40 | -    | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3356 | 1/1   | 0.98 | 0.17 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | DA    | 3215 | 1/1   | 0.90 | 0.56 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3028 | 1/1   | 0.95 | 0.33 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3285 | 1/1   | 0.96 | 0.20 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3266 | 1/1   | 0.93 | 0.31 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3281 | 1/1   | 0.91 | 0.21 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3297 | 1/1   | 0.48 | 0.69 | -    | 95,95,95,95                 | 0     |
| 59  | MG   | BA    | 3377 | 1/1   | 0.96 | 0.36 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3203 | 1/1   | 0.49 | 0.90 | -    | 97,97,97,97                 | 0     |
| 59  | MG   | DA    | 3166 | 1/1   | 0.74 | 0.12 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3126 | 1/1   | 0.87 | 0.33 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1725 | 1/1   | 0.83 | 0.26 | -    | 84,84,84,84                 | 0     |
| 59  | MG   | DA    | 3239 | 1/1   | 0.93 | 1.00 | -    | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3248 | 1/1   | 0.94 | 0.27 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3244 | 1/1   | 0.92 | 0.20 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3379 | 1/1   | 0.92 | 0.51 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3357 | 1/1   | 0.83 | 0.23 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3045 | 1/1   | 0.98 | 0.14 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3174 | 1/1   | 0.98 | 0.05 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | D5    | 101  | 1/1   | 0.95 | 0.14 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | DA    | 3225 | 1/1   | 0.96 | 0.76 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | AA    | 1610 | 1/1   | 0.93 | 0.09 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | DA    | 3223 | 1/1   | 0.89 | 0.17 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3075 | 1/1   | 0.94 | 0.29 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3263 | 1/1   | 0.98 | 0.16 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3009 | 1/1   | 0.98 | 0.25 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3273 | 1/1   | 0.93 | 0.21 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3219 | 1/1   | 0.90 | 0.17 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3096 | 1/1   | 0.99 | 0.11 | -    | 17,17,17,17                 | 0     |
| 59  | MG   | DA    | 3198 | 1/1   | 0.89 | 0.49 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3126 | 1/1   | 0.83 | 0.30 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3268 | 1/1   | 0.92 | 0.47 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | AA    | 1613 | 1/1   | 0.98 | 0.08 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | DA    | 3264 | 1/1   | 0.96 | 0.36 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3330 | 1/1   | 0.98 | 0.09 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3184 | 1/1   | 0.83 | 0.26 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3160 | 1/1   | 0.96 | 0.28 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | DA    | 3204 | 1/1   | 0.97 | 0.14 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3230 | 1/1   | 0.88 | 0.17 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1704 | 1/1   | 0.98 | 0.06 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | CA    | 1691 | 1/1   | 0.94 | 0.15 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3111 | 1/1   | 0.93 | 0.62 | -    | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3025 | 1/1   | 1.00 | 0.16 | -    | 5,5,5,5                     | 0     |
| 59  | MG   | DA    | 3011 | 1/1   | 0.92 | 0.42 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | CV    | 102  | 1/1   | 0.95 | 0.35 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3141 | 1/1   | 0.99 | 0.23 | -    | 1,1,1,1                     | 0     |
| 59  | MG   | DA    | 3018 | 1/1   | 0.97 | 0.17 | -    | 14,14,14,14                 | 0     |
| 59  | MG   | CA    | 1680 | 1/1   | 0.98 | 0.17 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3038 | 1/1   | 0.97 | 0.14 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | DA    | 3141 | 1/1   | 0.96 | 0.14 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3173 | 1/1   | 0.94 | 0.20 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | CA    | 1636 | 1/1   | 0.92 | 0.17 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | AA    | 1639 | 1/1   | 0.90 | 0.16 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3228 | 1/1   | 0.97 | 0.05 | -    | 16,16,16,16                 | 0     |
| 59  | MG   | DA    | 3080 | 1/1   | 0.90 | 0.17 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | CA    | 1635 | 1/1   | 0.99 | 0.28 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3179 | 1/1   | 0.96 | 0.15 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3284 | 1/1   | 0.95 | 0.37 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | DA    | 3175 | 1/1   | 0.87 | 0.54 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3220 | 1/1   | 0.96 | 0.52 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3252 | 1/1   | 0.93 | 0.35 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | CA    | 1671 | 1/1   | 0.86 | 0.30 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3068 | 1/1   | 0.96 | 0.22 | -    | 15,15,15,15                 | 0     |
| 59  | MG   | DA    | 3270 | 1/1   | 0.85 | 0.27 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3178 | 1/1   | 0.90 | 0.57 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3307 | 1/1   | 0.67 | 0.44 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | DA    | 3207 | 1/1   | 0.81 | 0.95 | -    | 69,69,69,69                 | 0     |
| 59  | MG   | CE    | 202  | 1/1   | 0.96 | 0.21 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | B5    | 101  | 1/1   | 0.96 | 0.47 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3214 | 1/1   | 0.94 | 0.15 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3187 | 1/1   | 0.96 | 0.37 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BD    | 301  | 1/1   | 0.97 | 0.16 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | AA    | 1658 | 1/1   | 0.93 | 0.58 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3067 | 1/1   | 0.92 | 0.37 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | AW    | 106  | 1/1   | 0.78 | 0.48 | -    | 94,94,94,94                 | 0     |
| 59  | MG   | BA    | 3249 | 1/1   | 0.87 | 0.61 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | AE    | 201  | 1/1   | 0.93 | 0.21 | -    | 87,87,87,87                 | 0     |
| 59  | MG   | DA    | 3229 | 1/1   | 0.87 | 0.25 | -    | 76,76,76,76                 | 0     |
| 59  | MG   | CA    | 1651 | 1/1   | 0.85 | 0.15 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3396 | 1/1   | 0.91 | 0.18 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3007 | 1/1   | 0.98 | 0.57 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3019 | 1/1   | 0.90 | 0.31 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | DA    | 3145 | 1/1   | 0.91 | 0.31 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3175 | 1/1   | 0.93 | 0.24 | -    | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1664 | 1/1   | 0.96 | 0.41 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3253 | 1/1   | 0.90 | 0.29 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3222 | 1/1   | 0.96 | 0.11 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3123 | 1/1   | 0.86 | 0.26 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3194 | 1/1   | 0.97 | 0.33 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3059 | 1/1   | 0.97 | 0.06 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | CA    | 1626 | 1/1   | 0.94 | 0.33 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3136 | 1/1   | 0.88 | 0.30 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | AA    | 1701 | 1/1   | 0.98 | 0.29 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3042 | 1/1   | 0.96 | 0.20 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3347 | 1/1   | 0.72 | 0.84 | -    | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3276 | 1/1   | 0.91 | 0.25 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3198 | 1/1   | 0.96 | 0.08 | -    | 16,16,16,16                 | 0     |
| 59  | MG   | DA    | 3105 | 1/1   | 0.97 | 0.22 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3114 | 1/1   | 0.91 | 0.35 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | AA    | 1706 | 1/1   | 0.99 | 0.29 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | CA    | 1603 | 1/1   | 0.79 | 0.45 | -    | 113,113,113,113             | 0     |
| 59  | MG   | CA    | 1662 | 1/1   | 0.97 | 0.08 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3242 | 1/1   | 0.95 | 0.17 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | DA    | 3269 | 1/1   | 0.95 | 0.16 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | AA    | 1621 | 1/1   | 0.83 | 0.37 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | AT    | 201  | 1/1   | 0.43 | 0.13 | -    | 92,92,92,92                 | 0     |
| 59  | MG   | CA    | 1618 | 1/1   | 0.88 | 0.47 | -    | 69,69,69,69                 | 0     |
| 59  | MG   | AA    | 1653 | 1/1   | 0.95 | 0.25 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3398 | 1/1   | 0.89 | 0.40 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3148 | 1/1   | 0.90 | 0.17 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | CA    | 1611 | 1/1   | 0.95 | 0.22 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3031 | 1/1   | 0.98 | 0.16 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3275 | 1/1   | 0.96 | 0.12 | -    | 93,93,93,93                 | 0     |
| 59  | MG   | BA    | 3211 | 1/1   | 0.94 | 0.18 | -    | 16,16,16,16                 | 0     |
| 59  | MG   | AX    | 104  | 1/1   | 0.90 | 0.27 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3271 | 1/1   | 0.78 | 0.16 | -    | 80,80,80,80                 | 0     |
| 59  | MG   | DA    | 3066 | 1/1   | 0.97 | 0.27 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | CA    | 1601 | 1/1   | 0.97 | 0.17 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3055 | 1/1   | 0.99 | 0.18 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3312 | 1/1   | 0.94 | 0.13 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3372 | 1/1   | 0.94 | 0.21 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3069 | 1/1   | 0.95 | 0.22 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | DA    | 3135 | 1/1   | 0.98 | 0.33 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1605 | 1/1   | 0.23 | 0.46 | -    | 99,99,99,99                 | 0     |
| 59  | MG   | BA    | 3146 | 1/1   | 0.94 | 0.36 | -    | 12,12,12,12                 | 0     |
| 59  | MG   | BA    | 3174 | 1/1   | 0.88 | 0.14 | -    | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3033 | 1/1   | 0.96 | 0.29 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | CA    | 1657 | 1/1   | 0.88 | 0.69 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | B0    | 102  | 1/1   | 0.86 | 0.32 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3179 | 1/1   | 0.91 | 0.33 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | CA    | 1653 | 1/1   | 0.92 | 0.15 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3243 | 1/1   | 0.95 | 0.29 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3022 | 1/1   | 0.93 | 0.17 | -    | 14,14,14,14                 | 0     |
| 59  | MG   | DE    | 301  | 1/1   | 0.98 | 0.20 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3144 | 1/1   | 0.91 | 0.57 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | CA    | 1613 | 1/1   | 0.95 | 0.07 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | AW    | 107  | 1/1   | 0.94 | 0.14 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3235 | 1/1   | 0.90 | 0.36 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3299 | 1/1   | 0.86 | 1.42 | -    | 85,85,85,85                 | 0     |
| 59  | MG   | DA    | 3193 | 1/1   | 0.88 | 0.18 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3290 | 1/1   | 0.63 | 0.17 | -    | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3104 | 1/1   | 0.97 | 0.11 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3171 | 1/1   | 0.81 | 0.46 | -    | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3085 | 1/1   | 0.97 | 0.41 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | CE    | 201  | 1/1   | 0.88 | 0.08 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3394 | 1/1   | 0.88 | 0.25 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3132 | 1/1   | 0.95 | 0.17 | -    | 87,87,87,87                 | 0     |
| 59  | MG   | BA    | 3365 | 1/1   | 0.94 | 0.15 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3071 | 1/1   | 0.98 | 0.18 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | DA    | 3247 | 1/1   | 0.62 | 0.35 | -    | 82,82,82,82                 | 0     |
| 59  | MG   | DA    | 3115 | 1/1   | 0.99 | 0.15 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3375 | 1/1   | 0.95 | 0.20 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3265 | 1/1   | 0.88 | 0.44 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | DA    | 3125 | 1/1   | 0.92 | 0.39 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3138 | 1/1   | 0.93 | 0.17 | -    | 17,17,17,17                 | 0     |
| 59  | MG   | AA    | 1643 | 1/1   | 0.87 | 0.20 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3208 | 1/1   | 0.90 | 0.20 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3044 | 1/1   | 0.98 | 0.28 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3363 | 1/1   | 0.93 | 0.26 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | AA    | 1638 | 1/1   | 0.91 | 0.18 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3151 | 1/1   | 0.96 | 0.13 | -    | 14,14,14,14                 | 0     |
| 59  | MG   | BA    | 3378 | 1/1   | 0.95 | 0.29 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | CA    | 1648 | 1/1   | 0.95 | 0.18 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BH    | 201  | 1/1   | 0.96 | 0.13 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | CA    | 1682 | 1/1   | 0.95 | 0.50 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3268 | 1/1   | 0.92 | 0.21 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | AA    | 1670 | 1/1   | 0.95 | 0.22 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3166 | 1/1   | 0.85 | 0.20 | -    | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3308 | 1/1   | 0.89 | 0.82 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3034 | 1/1   | 0.96 | 0.07 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3315 | 1/1   | 0.86 | 0.39 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3374 | 1/1   | 0.83 | 0.42 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3088 | 1/1   | 0.89 | 0.15 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3087 | 1/1   | 0.92 | 0.84 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3323 | 1/1   | 0.80 | 0.17 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3050 | 1/1   | 0.96 | 0.36 | -    | 70,70,70,70                 | 0     |
| 59  | MG   | CA    | 1666 | 1/1   | 0.89 | 0.08 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3339 | 1/1   | 0.94 | 0.39 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3252 | 1/1   | 0.89 | 0.12 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3329 | 1/1   | 0.96 | 0.09 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3111 | 1/1   | 0.98 | 0.26 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3145 | 1/1   | 0.95 | 0.32 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | AA    | 1692 | 1/1   | 0.98 | 0.05 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | AA    | 1618 | 1/1   | 0.94 | 0.23 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | AC    | 301  | 1/1   | 0.86 | 0.15 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3159 | 1/1   | 0.82 | 0.19 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3162 | 1/1   | 0.76 | 0.64 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3382 | 1/1   | 0.85 | 0.34 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3099 | 1/1   | 0.87 | 0.87 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3176 | 1/1   | 0.86 | 0.27 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1666 | 1/1   | 0.92 | 0.81 | -    | 75,75,75,75                 | 0     |
| 59  | MG   | DA    | 3163 | 1/1   | 0.89 | 0.61 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3152 | 1/1   | 0.98 | 0.39 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | AA    | 1688 | 1/1   | 0.89 | 0.26 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | CA    | 1612 | 1/1   | 0.81 | 0.50 | -    | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3328 | 1/1   | 0.97 | 0.21 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3072 | 1/1   | 0.99 | 0.23 | -    | 16,16,16,16                 | 0     |
| 59  | MG   | BA    | 3393 | 1/1   | 0.94 | 0.16 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3078 | 1/1   | 0.92 | 0.12 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | DA    | 3226 | 1/1   | 0.85 | 0.71 | -    | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3343 | 1/1   | 0.94 | 0.21 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1733 | 1/1   | 0.94 | 0.13 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3165 | 1/1   | 0.74 | 0.63 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3182 | 1/1   | 0.80 | 0.86 | -    | 81,81,81,81                 | 0     |
| 59  | MG   | AA    | 1648 | 1/1   | 0.87 | 0.24 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3020 | 1/1   | 0.95 | 0.26 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3086 | 1/1   | 0.97 | 0.16 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3195 | 1/1   | 0.94 | 0.15 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | AA    | 1730 | 1/1   | 0.95 | 0.51 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | DA    | 3254 | 1/1   | 0.89 | 0.17 | -    | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3303 | 1/1   | 0.79 | 0.86 | -    | 91,91,91,91                 | 0     |
| 59  | MG   | DA    | 3172 | 1/1   | 0.91 | 0.30 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3038 | 1/1   | 0.93 | 0.25 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | AA    | 1659 | 1/1   | 0.75 | 0.24 | -    | 73,73,73,73                 | 0     |
| 59  | MG   | CA    | 1621 | 1/1   | 0.90 | 0.40 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3027 | 1/1   | 0.87 | 0.24 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3146 | 1/1   | 0.92 | 0.20 | -    | 70,70,70,70                 | 0     |
| 59  | MG   | CA    | 1608 | 1/1   | 0.87 | 0.80 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3046 | 1/1   | 0.96 | 0.18 | -    | 15,15,15,15                 | 0     |
| 59  | MG   | DA    | 3067 | 1/1   | 0.98 | 0.27 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3051 | 1/1   | 0.96 | 0.22 | -    | 1,1,1,1                     | 0     |
| 59  | MG   | BA    | 3332 | 1/1   | 0.41 | 0.45 | -    | 105,105,105,105             | 0     |
| 59  | MG   | BA    | 3228 | 1/1   | 0.90 | 0.46 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | DA    | 3117 | 1/1   | 0.97 | 0.08 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3002 | 1/1   | 0.85 | 0.17 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3283 | 1/1   | 0.95 | 0.27 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3226 | 1/1   | 0.96 | 0.09 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | DA    | 3085 | 1/1   | 0.97 | 0.25 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3191 | 1/1   | 0.94 | 0.08 | -    | 77,77,77,77                 | 0     |
| 59  | MG   | AA    | 1650 | 1/1   | 0.99 | 0.20 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3143 | 1/1   | 0.99 | 0.27 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | DA    | 3259 | 1/1   | 0.94 | 0.36 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | AA    | 1662 | 1/1   | 0.93 | 0.22 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3185 | 1/1   | 0.84 | 0.33 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3084 | 1/1   | 0.87 | 0.14 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3272 | 1/1   | 0.95 | 0.52 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | DA    | 3220 | 1/1   | 0.87 | 0.18 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | CA    | 1649 | 1/1   | 0.93 | 0.09 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1608 | 1/1   | 0.94 | 0.07 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | AA    | 1723 | 1/1   | 0.88 | 0.14 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3122 | 1/1   | 0.97 | 0.20 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3210 | 1/1   | 0.88 | 0.25 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3120 | 1/1   | 0.88 | 0.15 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3351 | 1/1   | 0.80 | 0.30 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3119 | 1/1   | 0.91 | 0.16 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3300 | 1/1   | 0.95 | 0.13 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | DA    | 3267 | 1/1   | 0.96 | 0.28 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3219 | 1/1   | 0.79 | 0.26 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3241 | 1/1   | 0.94 | 0.27 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3280 | 1/1   | 0.93 | 0.37 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | CA    | 1690 | 1/1   | 0.96 | 0.14 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3072 | 1/1   | 0.97 | 0.29 | -    | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3287 | 1/1   | 0.93 | 0.57 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3138 | 1/1   | 0.95 | 0.12 | -    | 19,19,19,19                 | 0     |
| 59  | MG   | BA    | 3239 | 1/1   | 0.93 | 0.21 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3391 | 1/1   | 0.93 | 0.20 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | CA    | 1643 | 1/1   | 0.84 | 0.62 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3136 | 1/1   | 0.99 | 0.07 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1689 | 1/1   | 0.81 | 0.21 | -    | 73,73,73,73                 | 0     |
| 59  | MG   | AA    | 1724 | 1/1   | 0.86 | 0.36 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3310 | 1/1   | 0.88 | 0.37 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3289 | 1/1   | 0.96 | 0.18 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3059 | 1/1   | 0.99 | 0.03 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3036 | 1/1   | 0.97 | 0.32 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | CA    | 1641 | 1/1   | 0.93 | 0.15 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3362 | 1/1   | 0.85 | 0.35 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | CA    | 1679 | 1/1   | 0.90 | 0.18 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | AX    | 102  | 1/1   | 0.86 | 0.12 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3076 | 1/1   | 0.98 | 0.42 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3008 | 1/1   | 0.99 | 0.20 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3291 | 1/1   | 0.91 | 0.15 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3125 | 1/1   | 0.94 | 0.48 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | BX    | 101  | 1/1   | 0.70 | 0.53 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3047 | 1/1   | 0.97 | 0.17 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | DA    | 3168 | 1/1   | 0.89 | 0.26 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | CA    | 1688 | 1/1   | 0.90 | 0.14 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3248 | 1/1   | 0.94 | 0.46 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3364 | 1/1   | 0.97 | 0.18 | -    | 8,8,8,8                     | 0     |
| 59  | MG   | BA    | 3043 | 1/1   | 0.91 | 0.32 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3016 | 1/1   | 0.97 | 0.41 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1623 | 1/1   | 0.93 | 0.22 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3259 | 1/1   | 0.85 | 0.16 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3395 | 1/1   | 0.95 | 0.18 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3014 | 1/1   | 0.89 | 0.21 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | DA    | 3180 | 1/1   | 0.97 | 0.50 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3397 | 1/1   | 0.88 | 0.47 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3052 | 1/1   | 0.94 | 0.43 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3240 | 1/1   | 0.91 | 0.13 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3061 | 1/1   | 0.94 | 0.28 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | AA    | 1605 | 1/1   | 0.91 | 0.30 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3013 | 1/1   | 0.96 | 0.42 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1606 | 1/1   | 0.96 | 0.28 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1712 | 1/1   | 0.92 | 0.43 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3176 | 1/1   | 0.86 | 0.18 | -    | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3153 | 1/1   | 0.92 | 0.17 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | AA    | 1686 | 1/1   | 0.90 | 0.15 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3390 | 1/1   | 0.96 | 0.19 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | CA    | 1661 | 1/1   | 0.91 | 0.45 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3016 | 1/1   | 0.96 | 0.12 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3154 | 1/1   | 0.99 | 0.07 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3222 | 1/1   | 0.96 | 0.20 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3236 | 1/1   | 0.97 | 0.22 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | CA    | 1632 | 1/1   | 0.97 | 0.30 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3225 | 1/1   | 0.97 | 0.25 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | AA    | 1682 | 1/1   | 0.97 | 0.12 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | AH    | 201  | 1/1   | 0.97 | 0.29 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3234 | 1/1   | 0.85 | 0.41 | -    | 84,84,84,84                 | 0     |
| 59  | MG   | DA    | 3188 | 1/1   | 0.96 | 0.34 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | DA    | 3095 | 1/1   | 0.79 | 1.17 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3092 | 1/1   | 0.98 | 0.08 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | DA    | 3004 | 1/1   | 0.96 | 0.23 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3190 | 1/1   | 0.96 | 0.17 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | DA    | 3068 | 1/1   | 0.87 | 0.20 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3348 | 1/1   | 0.88 | 0.38 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | CA    | 1667 | 1/1   | 0.96 | 0.26 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | CA    | 1622 | 1/1   | 0.92 | 0.26 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3207 | 1/1   | 0.98 | 0.19 | -    | 24,24,24,24                 | 0     |
| 59  | MG   | AA    | 1711 | 1/1   | 0.81 | 0.27 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | DR    | 201  | 1/1   | 0.83 | 0.32 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3320 | 1/1   | 0.78 | 1.92 | -    | 89,89,89,89                 | 0     |
| 59  | MG   | BA    | 3262 | 1/1   | 0.97 | 0.23 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3039 | 1/1   | 0.98 | 0.24 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3026 | 1/1   | 0.91 | 0.29 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | DA    | 3036 | 1/1   | 0.98 | 0.35 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3049 | 1/1   | 0.87 | 0.14 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3102 | 1/1   | 0.92 | 0.31 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3183 | 1/1   | 0.67 | 0.11 | -    | 100,100,100,100             | 0     |
| 59  | MG   | DA    | 3189 | 1/1   | 0.83 | 1.16 | -    | 92,92,92,92                 | 0     |
| 59  | MG   | BA    | 3286 | 1/1   | 0.95 | 0.19 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3058 | 1/1   | 0.93 | 0.21 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3293 | 1/1   | 0.91 | 0.64 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3113 | 1/1   | 0.93 | 0.18 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1675 | 1/1   | 0.97 | 0.48 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3104 | 1/1   | 0.91 | 0.41 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1620 | 1/1   | 0.57 | 0.33 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3373 | 1/1   | 0.89 | 0.34 | -    | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1609 | 1/1   | 0.98 | 0.11 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | AA    | 1694 | 1/1   | 0.97 | 0.27 | -    | 24,24,24,24                 | 0     |
| 59  | MG   | BA    | 3200 | 1/1   | 0.93 | 0.21 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3277 | 1/1   | 0.96 | 0.32 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3272 | 1/1   | 0.89 | 0.31 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1699 | 1/1   | 0.84 | 0.41 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3212 | 1/1   | 0.88 | 0.43 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3118 | 1/1   | 0.97 | 0.25 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3309 | 1/1   | 0.91 | 0.05 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3139 | 1/1   | 0.94 | 0.15 | -    | 15,15,15,15                 | 0     |
| 59  | MG   | BA    | 3094 | 1/1   | 0.89 | 0.13 | -    | 12,12,12,12                 | 0     |
| 59  | MG   | BA    | 3037 | 1/1   | 0.85 | 0.46 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3080 | 1/1   | 0.97 | 0.24 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3392 | 1/1   | 0.84 | 0.30 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1617 | 1/1   | 0.89 | 0.09 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3127 | 1/1   | 0.83 | 0.24 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3275 | 1/1   | 0.91 | 0.35 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3064 | 1/1   | 0.93 | 0.28 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3376 | 1/1   | 0.91 | 0.91 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3076 | 1/1   | 0.93 | 0.29 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3031 | 1/1   | 0.94 | 0.23 | -    | 12,12,12,12                 | 0     |
| 59  | MG   | DA    | 3238 | 1/1   | 0.75 | 0.53 | -    | 101,101,101,101             | 0     |
| 59  | MG   | BA    | 3340 | 1/1   | 0.93 | 0.13 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3119 | 1/1   | 0.78 | 0.47 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3089 | 1/1   | 0.92 | 0.15 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3371 | 1/1   | 0.91 | 0.25 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3160 | 1/1   | 0.92 | 0.33 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | AA    | 1651 | 1/1   | 0.93 | 0.30 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3321 | 1/1   | 0.96 | 0.23 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1672 | 1/1   | 0.89 | 0.15 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3331 | 1/1   | 0.87 | 0.12 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1668 | 1/1   | 0.99 | 0.20 | -    | 194,194,194,194             | 0     |
| 59  | MG   | BA    | 3333 | 1/1   | 0.80 | 0.66 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3274 | 1/1   | 0.87 | 0.18 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3383 | 1/1   | 0.92 | 0.34 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | CA    | 1681 | 1/1   | 0.94 | 0.07 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1624 | 1/1   | 0.76 | 0.18 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3400 | 1/1   | 0.90 | 0.17 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3074 | 1/1   | 0.97 | 0.18 | -    | 12,12,12,12                 | 0     |
| 59  | MG   | AK    | 201  | 1/1   | 0.83 | 0.31 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3326 | 1/1   | 0.90 | 0.15 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3134 | 1/1   | 0.94 | 0.26 | -    | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1632 | 1/1   | 0.96 | 0.37 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3098 | 1/1   | 0.94 | 0.31 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3013 | 1/1   | 0.97 | 0.24 | -    | 6,6,6,6                     | 0     |
| 59  | MG   | CA    | 1692 | 1/1   | 0.90 | 0.38 | -    | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3389 | 1/1   | 0.89 | 0.20 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3261 | 1/1   | 0.86 | 0.19 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3270 | 1/1   | 0.83 | 0.27 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3305 | 1/1   | 0.90 | 0.29 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3149 | 1/1   | 0.96 | 0.44 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | AA    | 1715 | 1/1   | 0.94 | 0.14 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3282 | 1/1   | 0.96 | 0.22 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3256 | 1/1   | 0.88 | 0.18 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3264 | 1/1   | 0.97 | 0.27 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | DA    | 3217 | 1/1   | 0.78 | 0.39 | -    | 85,85,85,85                 | 0     |
| 59  | MG   | BA    | 3314 | 1/1   | 0.96 | 0.19 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3110 | 1/1   | 0.93 | 0.20 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3164 | 1/1   | 0.83 | 0.49 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3055 | 1/1   | 0.97 | 0.39 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3229 | 1/1   | 0.92 | 0.36 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3108 | 1/1   | 0.91 | 0.14 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3227 | 1/1   | 0.84 | 0.19 | -    | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3122 | 1/1   | 0.95 | 0.20 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3187 | 1/1   | 0.90 | 0.51 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3113 | 1/1   | 0.97 | 0.40 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1700 | 1/1   | 0.78 | 0.32 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3117 | 1/1   | 0.93 | 0.24 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3093 | 1/1   | 0.93 | 0.25 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3298 | 1/1   | 0.74 | 1.44 | -    | 178,178,178,178             | 0     |
| 59  | MG   | DA    | 3148 | 1/1   | 0.94 | 0.62 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3352 | 1/1   | 0.86 | 0.47 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | DA    | 3062 | 1/1   | 0.96 | 0.18 | -    | 24,24,24,24                 | 0     |
| 59  | MG   | CA    | 1650 | 1/1   | 0.96 | 0.43 | -    | 69,69,69,69                 | 0     |
| 59  | MG   | AA    | 1647 | 1/1   | 0.73 | 0.29 | -    | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3006 | 1/1   | 0.99 | 0.33 | -    | 16,16,16,16                 | 0     |
| 59  | MG   | BA    | 3237 | 1/1   | 0.85 | 0.47 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | AD    | 301  | 1/1   | 0.92 | 0.12 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3074 | 1/1   | 0.94 | 0.35 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | AA    | 1628 | 1/1   | 0.95 | 0.47 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | CA    | 1628 | 1/1   | 0.96 | 0.08 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | DA    | 3157 | 1/1   | 0.93 | 0.41 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3029 | 1/1   | 0.96 | 0.15 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3197 | 1/1   | 0.87 | 0.33 | -    | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3027 | 1/1   | 0.92 | 0.46 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | DA    | 3195 | 1/1   | 0.97 | 0.30 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1607 | 1/1   | 0.94 | 0.44 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | AA    | 1652 | 1/1   | 0.87 | 0.43 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3265 | 1/1   | 0.74 | 0.24 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | AF    | 201  | 1/1   | 0.91 | 0.18 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3399 | 1/1   | 0.96 | 0.19 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | AA    | 1604 | 1/1   | 0.94 | 0.30 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | AX    | 106  | 1/1   | 0.86 | 0.14 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3245 | 1/1   | 0.71 | 0.33 | -    | 86,86,86,86                 | 0     |
| 59  | MG   | BA    | 3313 | 1/1   | 0.93 | 0.42 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | CA    | 1668 | 1/1   | 0.94 | 0.08 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BB    | 201  | 1/1   | 0.98 | 0.07 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3197 | 1/1   | 0.89 | 0.36 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3318 | 1/1   | 0.96 | 0.35 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | CV    | 101  | 1/1   | 0.91 | 0.24 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | CX    | 102  | 1/1   | 0.92 | 0.51 | -    | 78,78,78,78                 | 0     |
| 59  | MG   | AO    | 101  | 1/1   | 0.90 | 0.12 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3253 | 1/1   | 0.82 | 0.22 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3302 | 1/1   | 0.86 | 0.15 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3367 | 1/1   | 0.94 | 0.44 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3221 | 1/1   | 0.95 | 0.39 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3260 | 1/1   | 0.94 | 0.28 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3127 | 1/1   | 0.94 | 0.28 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3263 | 1/1   | 0.96 | 0.43 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3244 | 1/1   | 0.93 | 0.17 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3034 | 1/1   | 0.94 | 0.33 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3169 | 1/1   | 0.94 | 0.14 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3227 | 1/1   | 0.86 | 0.15 | -    | 69,69,69,69                 | 0     |
| 59  | MG   | AA    | 1722 | 1/1   | 0.93 | 0.15 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3086 | 1/1   | 0.95 | 0.54 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | CA    | 1654 | 1/1   | 0.95 | 0.12 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1625 | 1/1   | 0.97 | 0.20 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3021 | 1/1   | 0.93 | 0.17 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | CA    | 1665 | 1/1   | 0.94 | 0.27 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3103 | 1/1   | 0.89 | 0.66 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1691 | 1/1   | 0.92 | 0.44 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3224 | 1/1   | 0.85 | 0.12 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3278 | 1/1   | 0.95 | 0.31 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3133 | 1/1   | 0.93 | 0.15 | -    | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3109 | 1/1   | 0.88 | 0.74 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3247 | 1/1   | 0.95 | 0.08 | -    | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1718 | 1/1   | 0.93 | 0.14 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | AA    | 1645 | 1/1   | 0.93 | 0.41 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3097 | 1/1   | 0.97 | 0.10 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | AA    | 1693 | 1/1   | 0.92 | 0.16 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3327 | 1/1   | 0.96 | 0.35 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3046 | 1/1   | 0.97 | 0.14 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3004 | 1/1   | 0.73 | 0.49 | -    | 81,81,81,81                 | 0     |
| 59  | MG   | BA    | 3294 | 1/1   | 0.68 | 1.08 | -    | 72,72,72,72                 | 0     |
| 59  | MG   | DA    | 3149 | 1/1   | 0.95 | 0.36 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | AY    | 101  | 1/1   | 0.94 | 0.17 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | DA    | 3006 | 1/1   | 0.97 | 0.31 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | DA    | 3186 | 1/1   | 0.80 | 0.16 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3271 | 1/1   | 0.93 | 0.49 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3242 | 1/1   | 0.97 | 0.58 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3094 | 1/1   | 0.94 | 0.24 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3158 | 1/1   | 0.95 | 0.12 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3170 | 1/1   | 0.93 | 0.26 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | CA    | 1645 | 1/1   | 0.90 | 0.05 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3338 | 1/1   | 0.94 | 0.07 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3171 | 1/1   | 0.95 | 0.51 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3032 | 1/1   | 0.98 | 0.15 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | CA    | 1683 | 1/1   | 0.76 | 0.55 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3380 | 1/1   | 0.95 | 0.19 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3019 | 1/1   | 0.99 | 0.19 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | DD    | 302  | 1/1   | 0.97 | 0.48 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3370 | 1/1   | 0.96 | 0.15 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | DA    | 3218 | 1/1   | 0.86 | 0.80 | -    | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3388 | 1/1   | 0.94 | 0.13 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3177 | 1/1   | 0.74 | 0.26 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3254 | 1/1   | 0.95 | 0.08 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3089 | 1/1   | 0.93 | 0.36 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | AA    | 1707 | 1/1   | 0.71 | 0.55 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3071 | 1/1   | 0.97 | 0.05 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3131 | 1/1   | 0.93 | 0.84 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3024 | 1/1   | 0.97 | 0.17 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1710 | 1/1   | 0.54 | 0.65 | -    | 113,113,113,113             | 0     |
| 59  | MG   | BA    | 3028 | 1/1   | 0.86 | 0.22 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3180 | 1/1   | 0.94 | 0.35 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3231 | 1/1   | 0.94 | 0.21 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3162 | 1/1   | 0.93 | 0.11 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | AA    | 1696 | 1/1   | 0.98 | 0.20 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1635 | 1/1   | 0.88 | 0.21 | -    | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1655 | 1/1   | 0.86 | 0.40 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3304 | 1/1   | 0.96 | 0.46 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3060 | 1/1   | 0.96 | 0.13 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | DA    | 3255 | 1/1   | 0.95 | 0.15 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | AA    | 1671 | 1/1   | 0.90 | 0.18 | -    | 83,83,83,83                 | 0     |
| 59  | MG   | DA    | 3140 | 1/1   | 0.92 | 0.41 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1695 | 1/1   | 0.87 | 0.17 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3102 | 1/1   | 0.89 | 0.13 | -    | 84,84,84,84                 | 0     |
| 59  | MG   | CA    | 1672 | 1/1   | 0.57 | 0.27 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3156 | 1/1   | 0.96 | 0.29 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3292 | 1/1   | 0.90 | 0.31 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | CA    | 1647 | 1/1   | 0.94 | 0.43 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | DA    | 3078 | 1/1   | 0.88 | 0.24 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1615 | 1/1   | 0.99 | 0.21 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3161 | 1/1   | 0.93 | 0.50 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | CA    | 1689 | 1/1   | 0.85 | 0.15 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3324 | 1/1   | 0.93 | 0.45 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3048 | 1/1   | 0.97 | 0.10 | -    | 6,6,6,6                     | 0     |
| 59  | MG   | DA    | 3235 | 1/1   | 0.84 | 0.23 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | CA    | 1617 | 1/1   | 0.93 | 0.28 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | DA    | 3240 | 1/1   | 0.88 | 0.19 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3041 | 1/1   | 0.99 | 0.21 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3003 | 1/1   | 0.88 | 0.39 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | CA    | 1644 | 1/1   | 0.77 | 0.80 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | AW    | 101  | 1/1   | 0.74 | 0.43 | -    | 135,135,135,135             | 0     |
| 59  | MG   | DA    | 3199 | 1/1   | 0.93 | 0.50 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1728 | 1/1   | 0.93 | 0.11 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3232 | 1/1   | 0.86 | 0.32 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | DA    | 3058 | 1/1   | 0.96 | 0.07 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3231 | 1/1   | 0.85 | 0.07 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3172 | 1/1   | 0.97 | 0.39 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3234 | 1/1   | 0.93 | 0.33 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3335 | 1/1   | 0.90 | 0.42 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3319 | 1/1   | 0.94 | 0.41 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3366 | 1/1   | 0.88 | 0.40 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BP    | 201  | 1/1   | 0.95 | 0.11 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | AA    | 1702 | 1/1   | 0.92 | 0.52 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3201 | 1/1   | 0.95 | 0.12 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | AA    | 1719 | 1/1   | 0.92 | 0.29 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1676 | 1/1   | 0.97 | 0.17 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | CA    | 1619 | 1/1   | 0.89 | 0.43 | -    | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3322 | 1/1   | 0.94 | 0.67 | -    | 147,147,147,147             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1729 | 1/1   | 0.81 | 0.26 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3042 | 1/1   | 0.94 | 0.29 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | AK    | 202  | 1/1   | 0.71 | 0.30 | -    | 90,90,90,90                 | 0     |
| 59  | MG   | DA    | 3210 | 1/1   | 0.87 | 0.47 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | AA    | 1601 | 1/1   | 0.96 | 0.08 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1654 | 1/1   | 0.87 | 0.25 | -    | 100,100,100,100             | 0     |
| 59  | MG   | DA    | 3181 | 1/1   | 0.64 | 0.25 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3211 | 1/1   | 0.69 | 1.14 | -    | 78,78,78,78                 | 0     |
| 59  | MG   | AA    | 1642 | 1/1   | 0.92 | 0.12 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3354 | 1/1   | 0.94 | 0.11 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3369 | 1/1   | 0.94 | 0.28 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3040 | 1/1   | 0.98 | 0.07 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | CA    | 1602 | 1/1   | 0.96 | 0.37 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3053 | 1/1   | 0.86 | 0.19 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | AA    | 1660 | 1/1   | 0.93 | 0.41 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3084 | 1/1   | 0.90 | 0.26 | -    | 19,19,19,19                 | 0     |
| 59  | MG   | DA    | 3073 | 1/1   | 0.96 | 0.22 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3358 | 1/1   | 0.97 | 0.09 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3251 | 1/1   | 0.81 | 0.17 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3246 | 1/1   | 0.90 | 0.51 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3350 | 1/1   | 0.93 | 0.13 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3140 | 1/1   | 0.98 | 0.04 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3070 | 1/1   | 0.95 | 0.08 | -    | 14,14,14,14                 | 0     |
| 59  | MG   | BA    | 3196 | 1/1   | 0.88 | 0.29 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1670 | 1/1   | 0.73 | 0.29 | -    | 67,67,67,67                 | 0     |
| 59  | MG   | AA    | 1667 | 1/1   | 0.75 | 0.38 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3170 | 1/1   | 0.86 | 0.14 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3325 | 1/1   | 0.94 | 0.14 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | AL    | 201  | 1/1   | 0.94 | 0.46 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3213 | 1/1   | 0.75 | 0.65 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3026 | 1/1   | 0.98 | 0.16 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3118 | 1/1   | 0.96 | 0.16 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | CA    | 1609 | 1/1   | 0.93 | 0.48 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3129 | 1/1   | 0.98 | 0.40 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3342 | 1/1   | 0.97 | 0.21 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | DA    | 3065 | 1/1   | 0.92 | 0.32 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1636 | 1/1   | 0.97 | 0.25 | -    | 21,21,21,21                 | 0     |
| 59  | MG   | DA    | 3032 | 1/1   | 0.99 | 0.09 | -    | 9,9,9,9                     | 0     |
| 59  | MG   | BA    | 3349 | 1/1   | 0.91 | 0.18 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3030 | 1/1   | 0.85 | 0.10 | -    | 17,17,17,17                 | 0     |
| 59  | MG   | DA    | 3121 | 1/1   | 0.85 | 0.18 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3064 | 1/1   | 0.99 | 0.15 | -    | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3100 | 1/1   | 0.92 | 0.37 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3273 | 1/1   | 0.70 | 0.96 | -    | 106,106,106,106             | 0     |
| 59  | MG   | DA    | 3029 | 1/1   | 0.94 | 0.34 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1708 | 1/1   | 0.98 | 0.04 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3163 | 1/1   | 0.96 | 0.12 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3159 | 1/1   | 0.96 | 0.14 | -    | 16,16,16,16                 | 0     |
| 59  | MG   | AX    | 107  | 1/1   | 0.74 | 0.58 | -    | 80,80,80,80                 | 0     |
| 59  | MG   | DA    | 3142 | 1/1   | 0.94 | 0.15 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3143 | 1/1   | 0.93 | 0.25 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3051 | 1/1   | 0.93 | 0.45 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1705 | 1/1   | 0.98 | 0.10 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | CA    | 1675 | 1/1   | 0.74 | 0.50 | -    | 150,150,150,150             | 0     |
| 59  | MG   | DA    | 3060 | 1/1   | 0.97 | 0.12 | -    | 16,16,16,16                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.