



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4V90  
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Deposited on : 2014-02-22  
Resolution : 2.95 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 : rb-20030736  
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) : rb-20030736

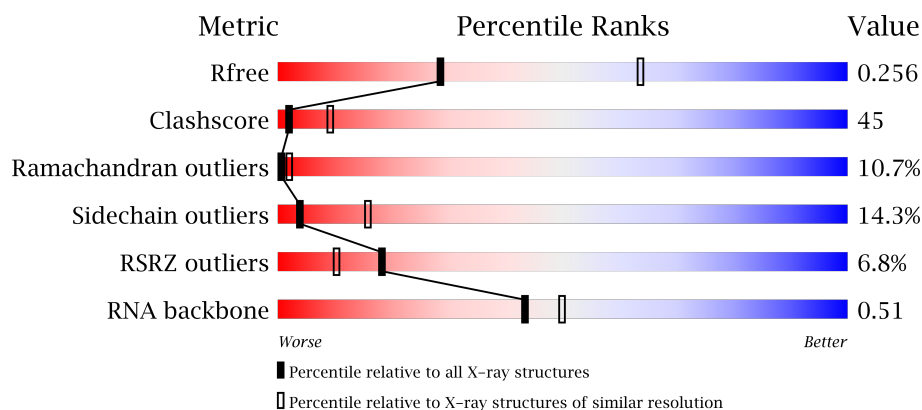
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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                      | 2395 (3.00-2.92)                                      |
| Clashscore            | 112137                      | 2773 (3.00-2.92)                                      |
| Ramachandran outliers | 110173                      | 2680 (3.00-2.92)                                      |
| Sidechain outliers    | 110143                      | 2683 (3.00-2.92)                                      |
| RSRZ outliers         | 101464                      | 2421 (3.00-2.92)                                      |
| RNA backbone          | 2435                        | 1008 (3.30-2.62)                                      |

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    | 1519   | <div> <div>3%</div> <div>33%</div> <div>47%</div> <div>19%</div> <div>.</div> </div>                |
| 2   | AB    | 256    | <div> <div>7%</div> <div>21%</div> <div>49%</div> <div>18%</div> <div>.</div> <div>8%</div> </div>  |
| 3   | AC    | 239    | <div> <div>4%</div> <div>23%</div> <div>44%</div> <div>18%</div> <div>.</div> <div>13%</div> </div> |
| 4   | AD    | 209    | <div> <div>2%</div> <div>45%</div> <div>45%</div> <div>9%</div> <div>.</div> </div>                 |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | AE    | 162    |                  |
| 6   | AF    | 101    |                  |
| 7   | AG    | 156    |                  |
| 8   | AH    | 138    |                  |
| 9   | AI    | 128    |                  |
| 10  | AJ    | 105    |                  |
| 11  | AK    | 129    |                  |
| 12  | AL    | 132    |                  |
| 13  | AM    | 126    |                  |
| 14  | AN    | 61     |                  |
| 15  | AO    | 89     |                  |
| 16  | AP    | 88     |                  |
| 17  | AQ    | 105    |                  |
| 18  | AR    | 88     |                  |
| 19  | AS    | 93     |                  |
| 20  | AT    | 106    |                  |
| 21  | AU    | 27     |                  |
| 22  | AV    | 76     |                  |
| 23  | AX    | 9      |                  |
| 24  | AY    | 691    |                  |
| 25  | B0    | 84     |                  |
| 26  | B1    | 97     |                  |
| 27  | B2    | 71     |                  |
| 28  | B3    | 60     |                  |
| 29  | B4    | 71     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 30  | B5    | 59     |                  |
| 31  | B6    | 53     |                  |
| 32  | B7    | 48     |                  |
| 33  | B8    | 64     |                  |
| 34  | B9    | 37     |                  |
| 35  | BA    | 2915   |                  |
| 36  | BB    | 122    |                  |
| 37  | BC    | 228    |                  |
| 38  | BD    | 275    |                  |
| 39  | BE    | 206    |                  |
| 40  | BF    | 210    |                  |
| 41  | BG    | 181    |                  |
| 42  | BH    | 180    |                  |
| 43  | BJ    | 130    |                  |
| 44  | BK    | 140    |                  |
| 45  | BL    | 71     |                  |
| 46  | BN    | 140    |                  |
| 47  | BO    | 122    |                  |
| 48  | BP    | 149    |                  |
| 49  | BQ    | 141    |                  |
| 50  | BR    | 117    |                  |
| 51  | BS    | 111    |                  |
| 52  | BT    | 146    |                  |
| 53  | BU    | 117    |                  |
| 54  | BV    | 101    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 55  | BW    | 113    |                  |
| 56  | BX    | 95     |                  |
| 57  | BY    | 109    |                  |
| 58  | BZ    | 205    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 59  | MG   | AA    | 1604 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1615 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1616 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1623 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1625 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1636 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1638 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1639 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1645 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1649 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1665 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1671 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1677 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1678 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1684 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1686 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1690 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1692 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1700 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1704 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1715 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1724 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1729 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1733 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1741 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1756 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1760 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1762 | -         | -        | -       | X                |
| 59  | MG   | AA    | 1777 | -         | -        | -       | X                |
| 59  | MG   | B0    | 101  | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 59  | MG   | BA    | 3004 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3006 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3007 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3024 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3039 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3043 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3044 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3048 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3051 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3052 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3053 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3056 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3071 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3075 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3077 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3078 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3082 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3084 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3087 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3088 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3091 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3094 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3097 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3098 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3104 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3108 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3109 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3110 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3111 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3113 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3116 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3120 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3125 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3127 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3129 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3139 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3145 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3149 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3153 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3154 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3169 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3172 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 59  | MG   | BA    | 3174 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3176 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3180 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3181 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3184 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3189 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3196 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3199 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3206 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3207 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3209 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3210 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3214 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3228 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3236 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3248 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3257 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3258 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3266 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3271 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3277 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3279 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3282 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3295 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3298 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3310 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3312 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3313 | -         | -        | -       | X                |
| 59  | MG   | BA    | 3315 | -         | -        | -       | X                |
| 60  | ZN   | AD    | 301  | -         | -        | -       | X                |
| 61  | GCP  | AY    | 701  | -         | -        | X       | -                |

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 153829 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    | 1507     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32391 | 14418 | 6002 | 10465 | 1506 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference |
|-------|---------|----------|--------|-----------|-----------|
| AA    | 1030    | C        | -      | insertion | GB 48256  |
| AA    | 1034    | G        | -      | insertion | GB 48256  |
| AA    | 1245    | A        | -      | insertion | GB 48256  |
| AA    | 1246    | C        | -      | insertion | GB 48256  |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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     |
|     |       |          | 1010  | 639 | 197 | 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 119      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 938   | 579 | 194 | 163 | 2 |         |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | AN    | 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |  |         |         |       |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 88       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 692   | 440 | 128 | 122 | 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 |         |         |       |

- 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 |  |         |         |       |

- Molecule 22 is a RNA chain called RNA (77-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | AV    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1619  | 723 | 291 | 530 | 75 |         |         |       |

- Molecule 23 is a RNA chain called 5'-R(\*UP\*AP\*AP\*AP\*AP\*AP\*UP\*GP\*UP)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 23  | AX    | 9        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 188   | 86 | 34 | 60 | 8 |         |         |       |

- Molecule 24 is a protein called ELONGATION FACTOR G.

| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 24  | AY    | 687      | Total | C    | N   | O    | S  | 0       | 0       | 1     |
|     |       |          | 5376  | 3412 | 922 | 1022 | 20 |         |         |       |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | B0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | B1    | 94       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 732   | 460 | 146 | 125 | 1 |         |         |       |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | B2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | B3    | 60       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 468   | 298 | 91 | 78 | 1 |         |         |       |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | B4    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 364 | 108 | 104 | 5 |         |         |       |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | B5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | B6    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 433   | 270 | 88 | 71 | 4 |         |         |       |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32  | B7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 419   | 257 | 104 | 56 | 2 |         |         |       |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33  | B8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 508   | 326 | 102 | 78 | 2 |         |         |       |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 34  | B9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 35  | BA    | 2901     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62476 | 27807 | 11683 | 20086 | 2900 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| BA    | 2155    | G        | A      | conflict | GB 55771382 |

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 36  | BB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |

- Molecule 37 is a protein called RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 37  | BC    | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1735  | 1096 | 318 | 318 | 3 |         |         |       |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 38  | BD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2145  | 1353 | 428 | 361 | 3 |         |         |       |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1564  | 988 | 300 | 270 | 6 |         |         |       |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 40  | BF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1624  | 1035 | 304 | 282 | 3 |         |         |       |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BG    | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1459  | 931 | 266 | 258 | 4 |         |         |       |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BH    | 176      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1345  | 853 | 253 | 237 | 2 |         |         |       |

- Molecule 43 is a protein called CHAIN J.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43  | BJ    | 130      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 654   | 393 | 130 | 131 |         |         |       |

- Molecule 44 is a protein called CHAIN K.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 44  | BK    | 140      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 701   | 420 | 140 | 141 |         |         |       |

- Molecule 45 is a protein called CHAIN L.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 45  | BL    | 71       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 356   | 213 | 71 | 72 |         |         |       |

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BN    | 139      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1105  | 712 | 207 | 182 | 4 |         |         |       |

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | BP    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1114  | 692 | 227 | 193 | 2 |         |         |       |

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | BQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 50  | BR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 51  | BS    | 99       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 771   | 486 | 155 | 130 |  |         |         |       |

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | BT    | 138      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1142  | 710 | 235 | 196 | 1 |         |         |       |

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | BU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 604 | 202 | 151 | 1 |         |         |       |

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | BV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55  | BW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56  | BX    | 93       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 726   | 471 | 132 | 123 |   |         |         |       |

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | BY    | 101      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 776   | 500 | 149 | 123 | 4 |         |         |       |

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58  | BZ    | 185      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1468  | 936 | 262 | 268 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 59  | B5    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | BU    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | BA    | 320      | Total | Mg  | 0       | 0       |
|     |       |          | 320   | 320 |         |         |

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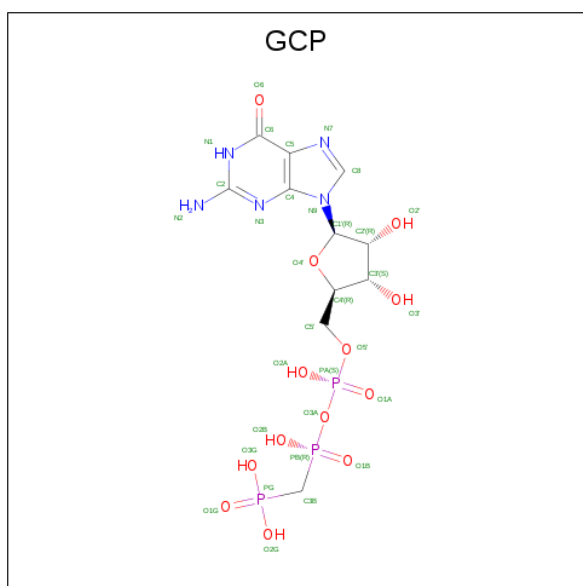
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| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 59  | AA    | 198      | Total | Mg  | 0       | 0       |
|     |       |          | 198   | 198 |         |         |
| 59  | B0    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AY    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | BC    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 60  | B9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 60  | AD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 60  | AN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 61 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

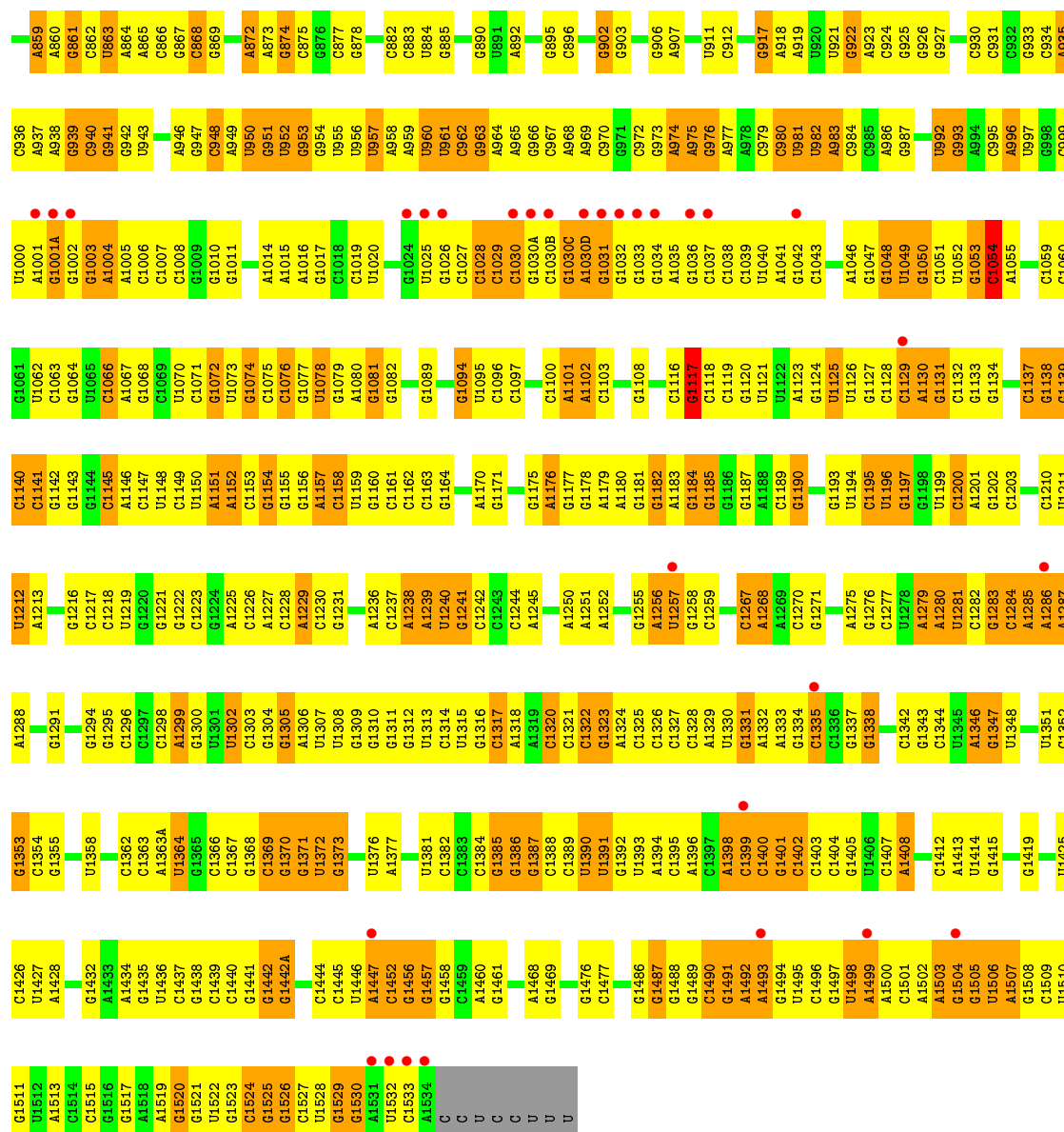


| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 61  | AY    | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |         |

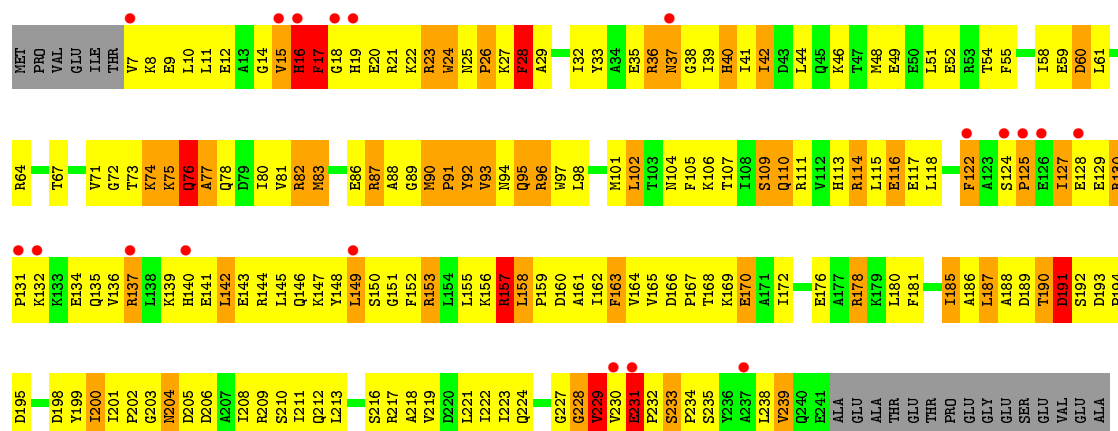
- Molecule 62 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 62  | AY    | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

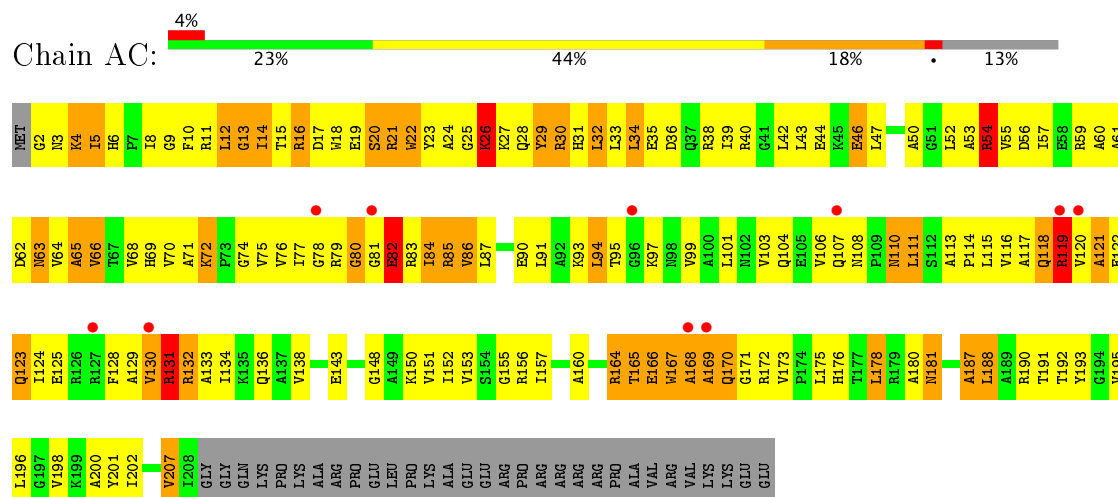




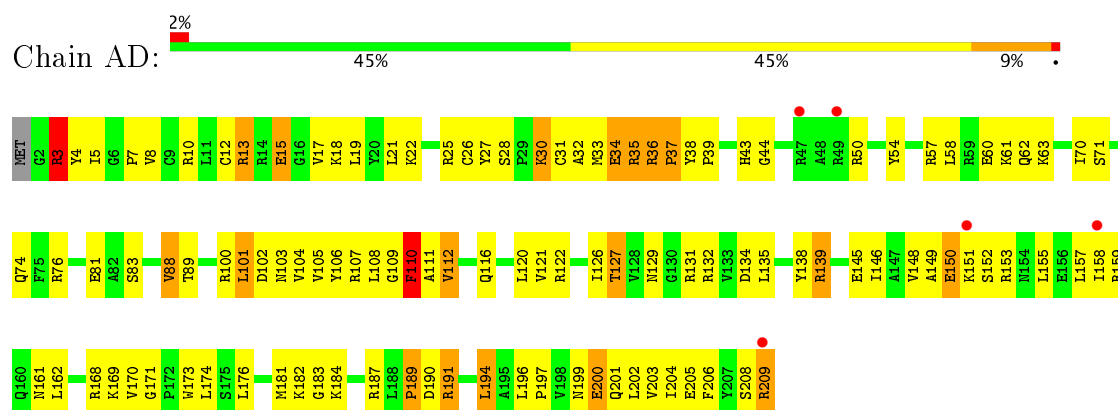
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



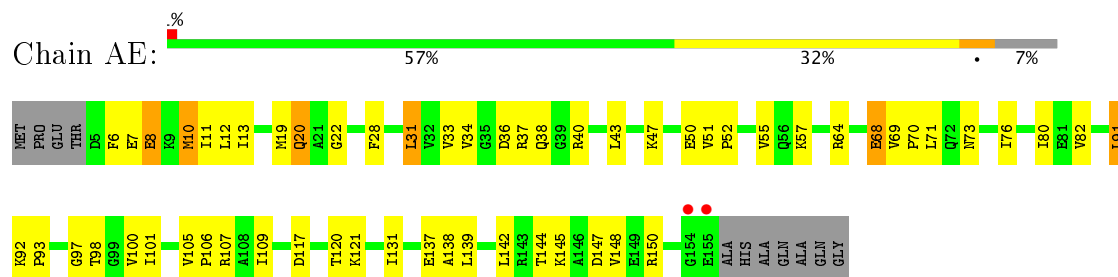
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



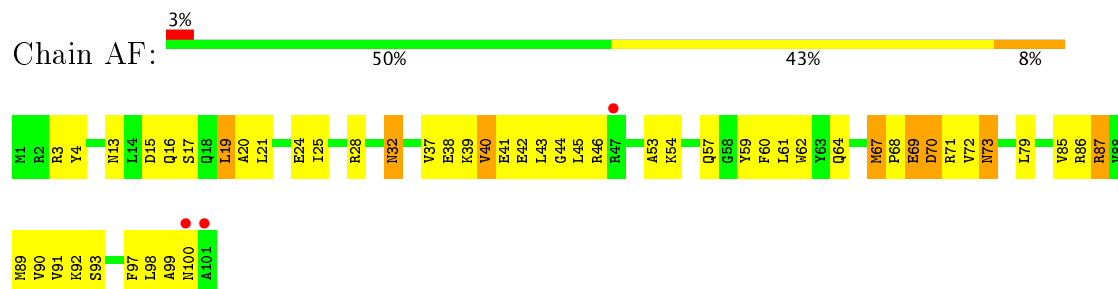
- Molecule 4: 30S RIBOSOMAL PROTEIN S4



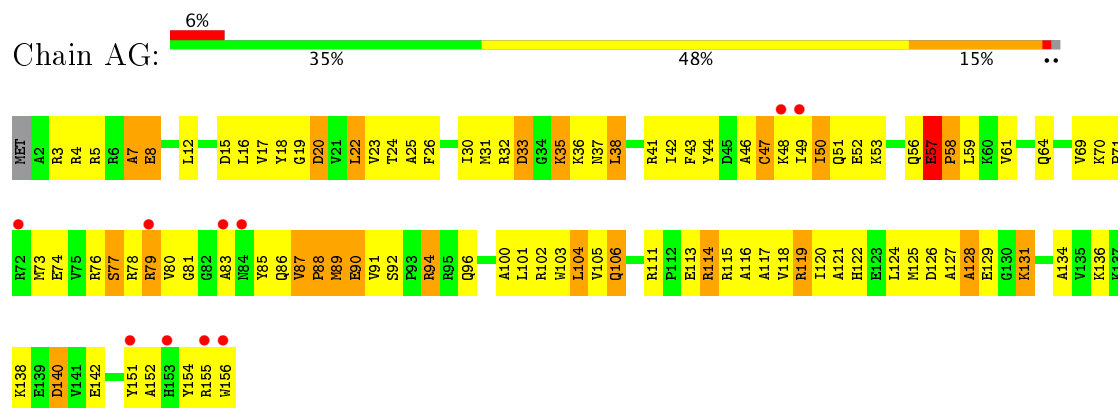
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



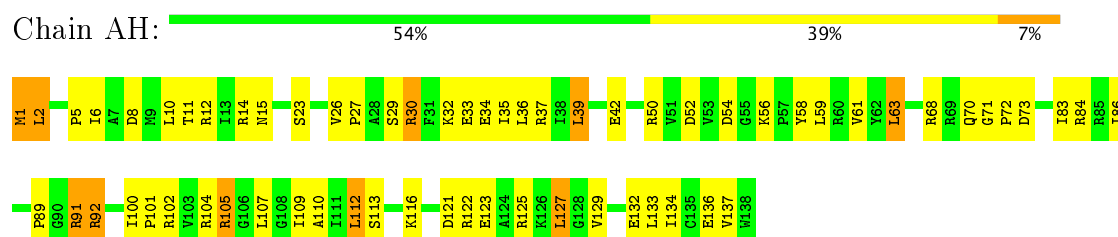
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



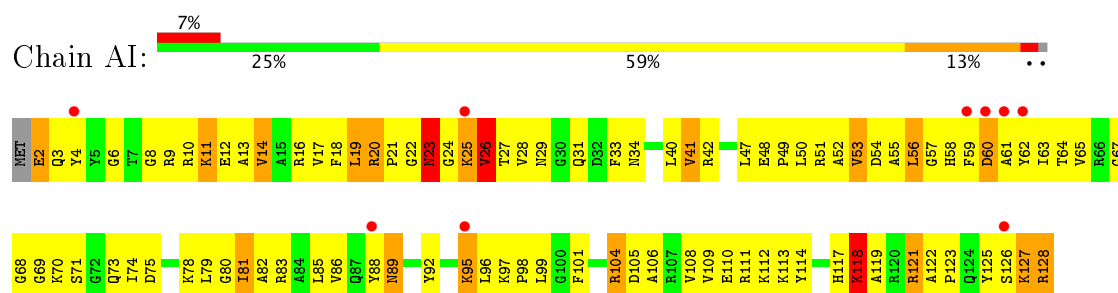
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



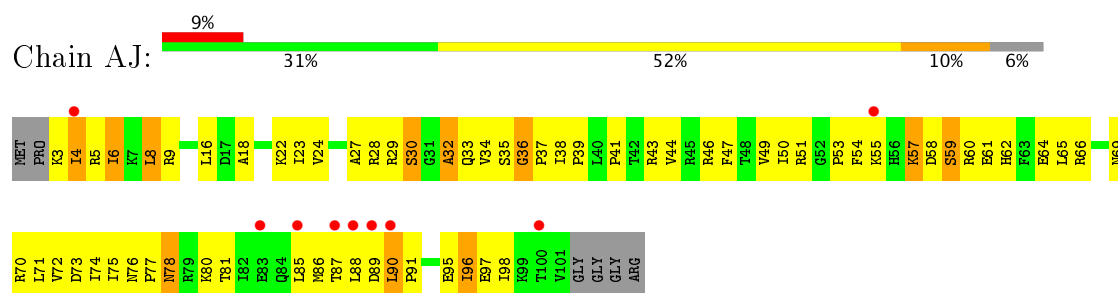
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



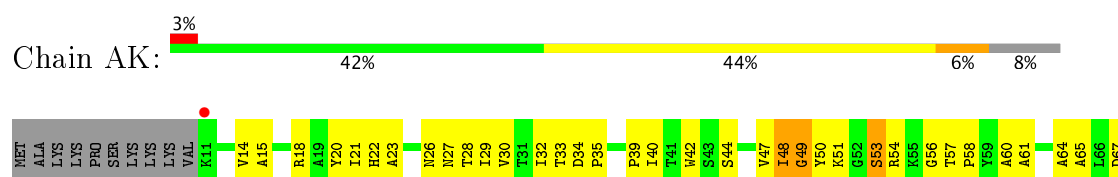
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

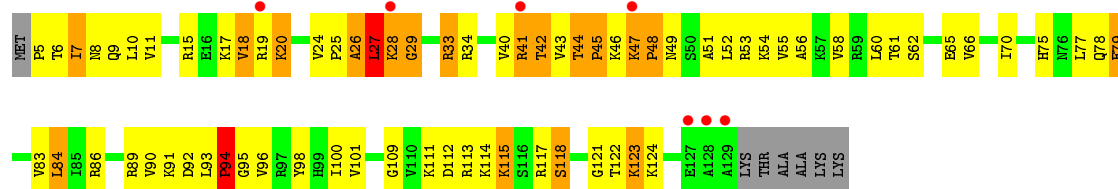


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

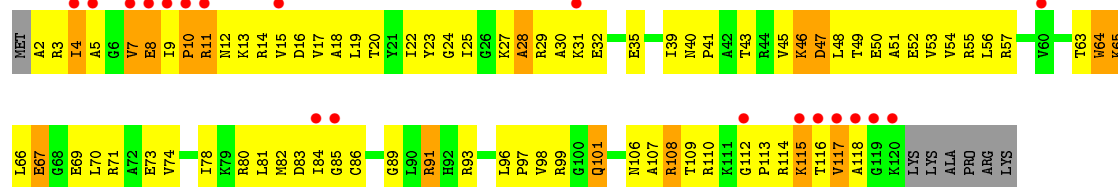




• Molecule 12: 30S RIBOSOMAL PROTEIN S12



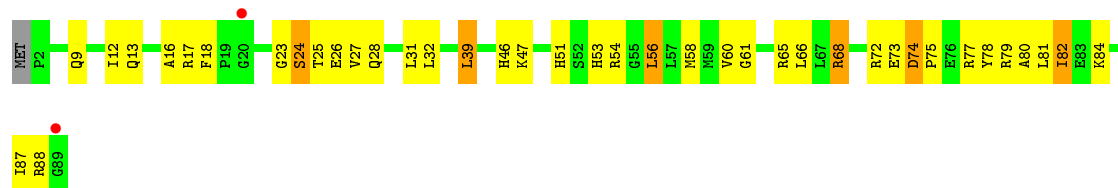
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



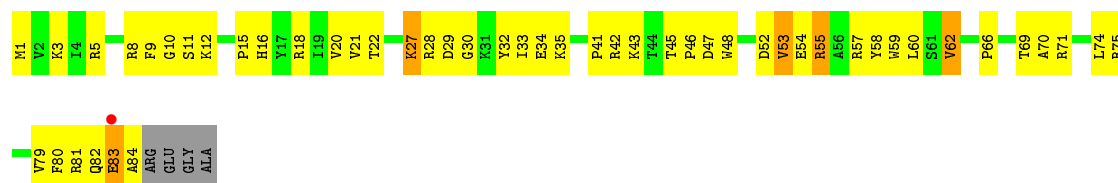
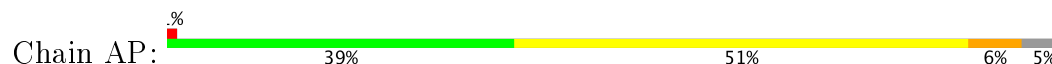
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

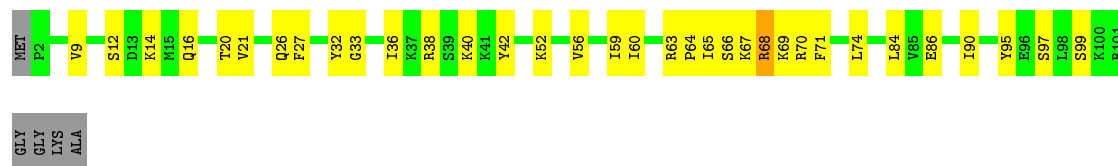


• Molecule 16: 30S RIBOSOMAL PROTEIN S16



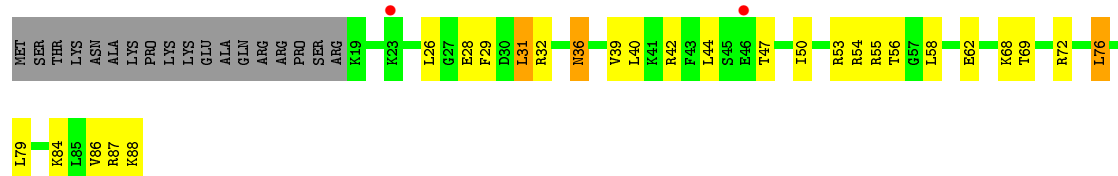
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 



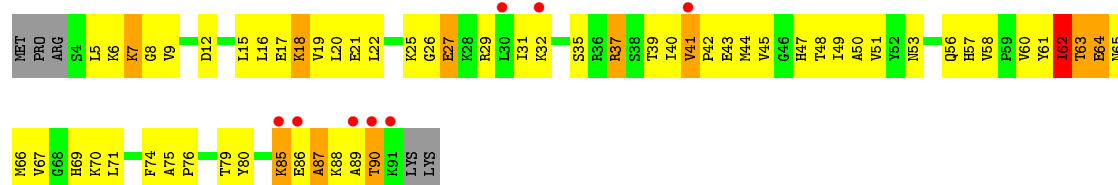
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 



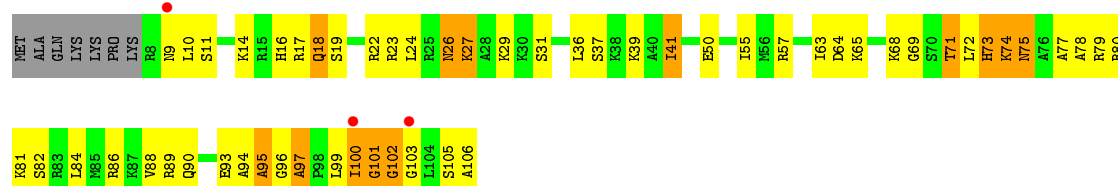
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS: 



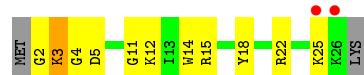
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT: 




- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU: 

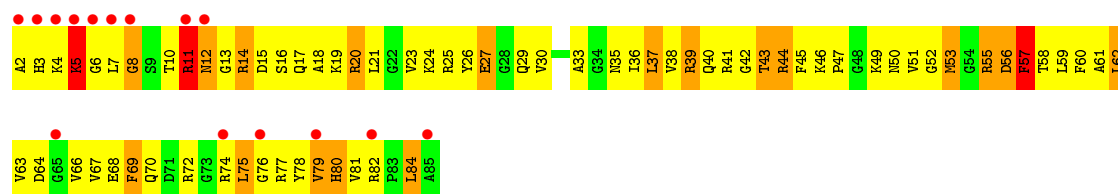


- Molecule 22: RNA (77-MER)

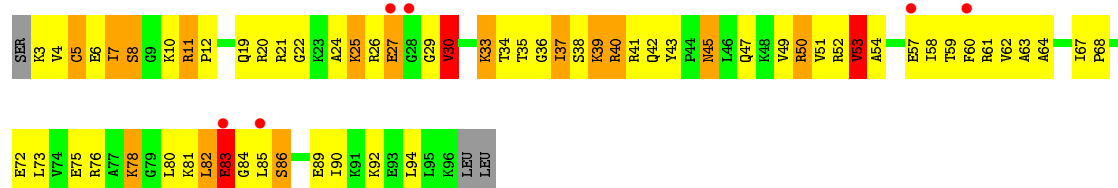
Chain AV: 



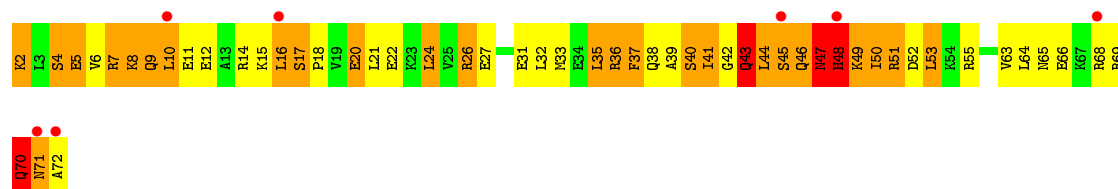
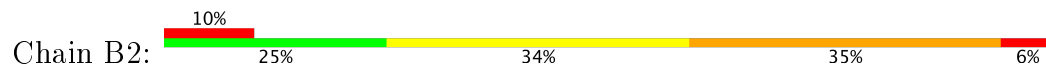




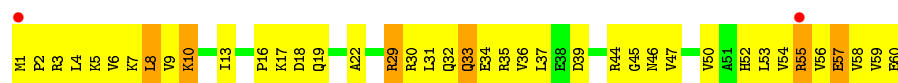
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



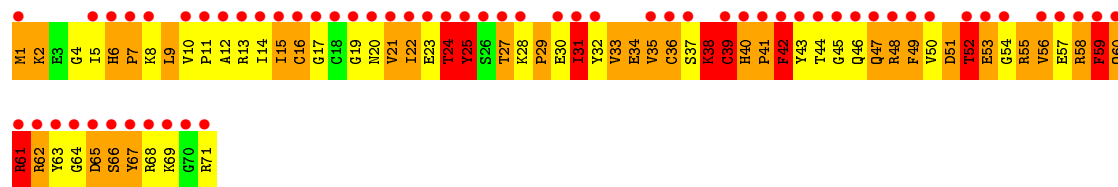
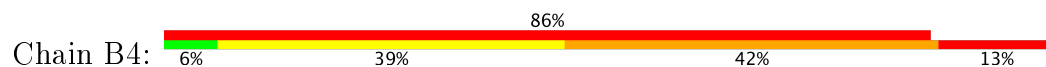
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30



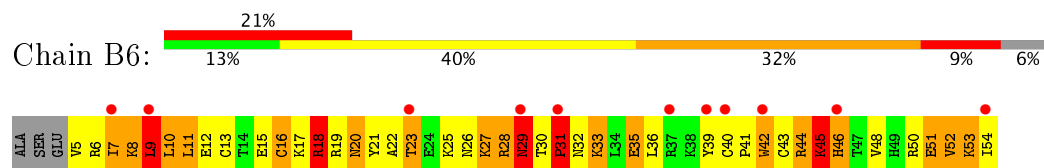
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



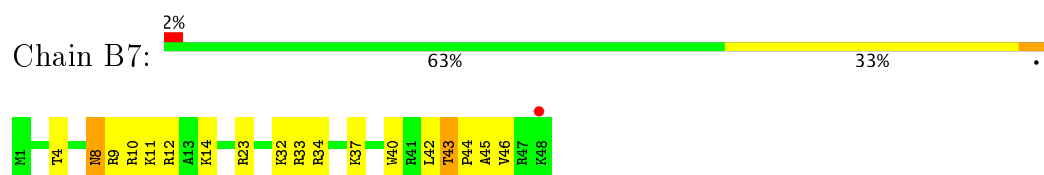
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



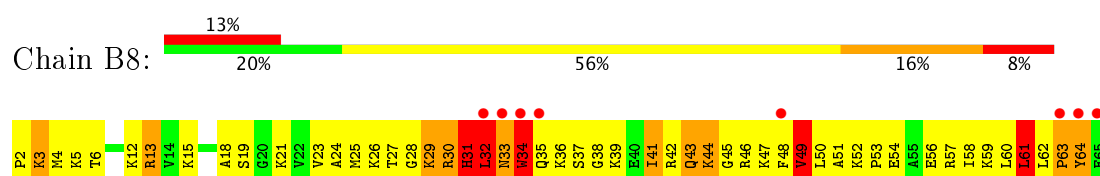
- Molecule 31: 50S RIBOSOMAL PROTEIN L33



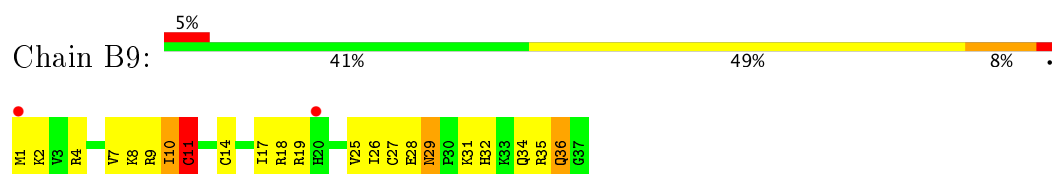
● Molecule 32: 50S RIBOSOMAL PROTEIN L34



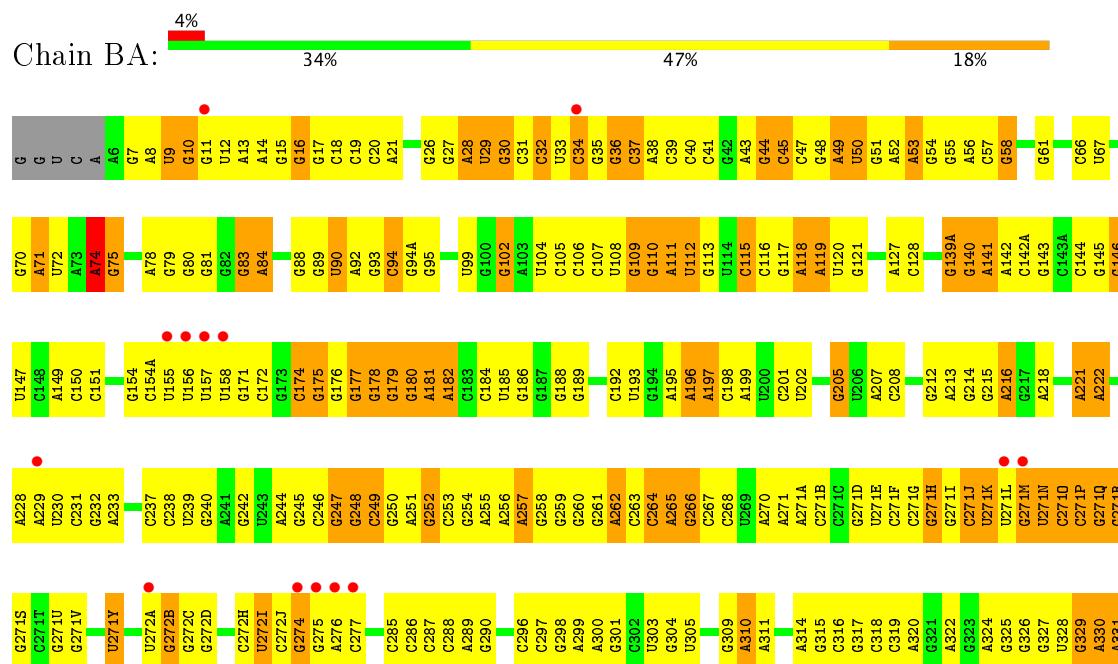
● Molecule 33: 50S RIBOSOMAL PROTEIN L35



- Molecule 34: 50S RIBOSOMAL PROTEIN L36

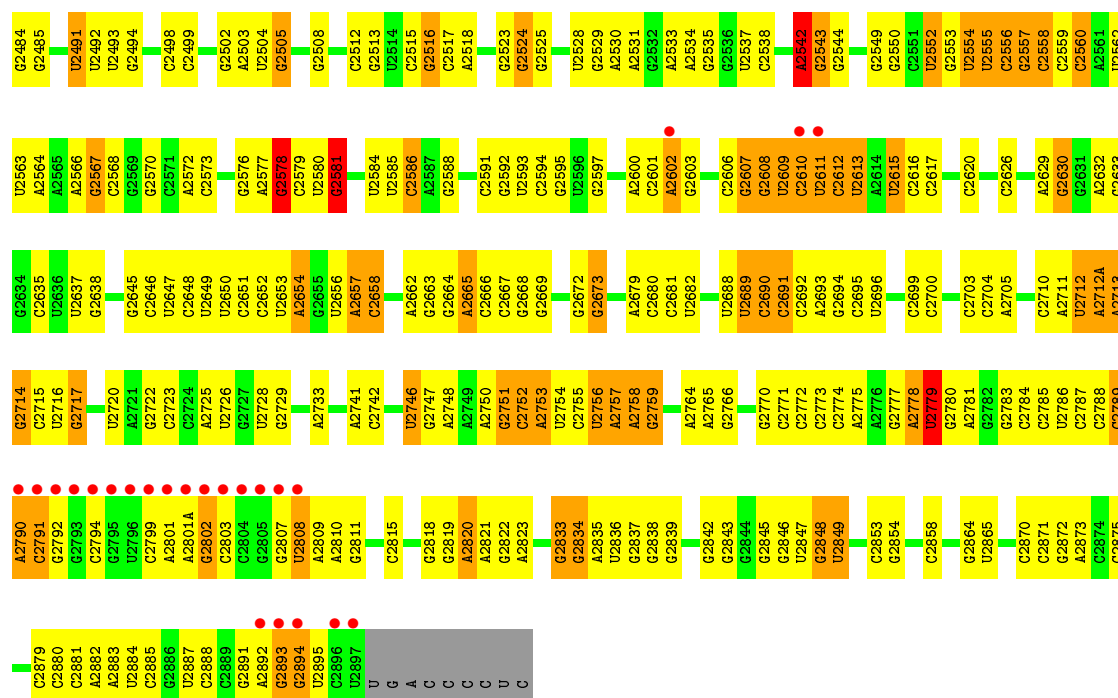


- Molecule 35: 23S RIBOSOMAL RNA

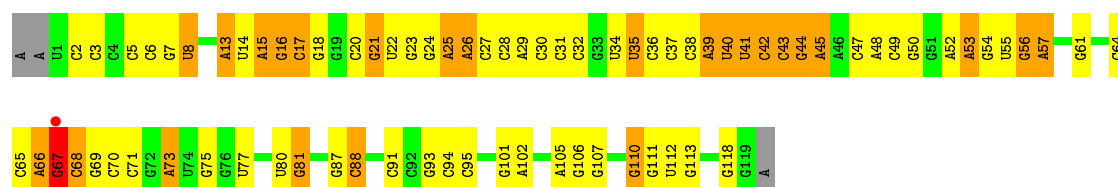


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |        |       |       |       |       |       |        |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|
| G1332 | C1333 | A1336 | G1337 | G1344 | G1345 | G1348 | G1349 | G1350 | C1351 | G1352 | A1353 | G1358 | A1359 | A1360 | G1361 | G1362 | G1363 | G1364 | A1365 | G1368 | G1374  | G1375 | G1376 | G1377 | A1378 | A1379 | G1380  | G1381 | G1382 | C1383 | A1384 | G1385 | G1386 | C1387 | U1396 | A1403 | U1404 | U1405 | U1406 | C1407 | C1408 | C1411 | A1412 | G1413 | G1414 | U1415 | G1416 | C1417 | G1418 |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| C1257 | C1258 | G1259 | G1260 | U1263 | G1264 | A1265 | U1267 | A1268 | A1269 | U1270 | G1271 | G1272 | C1273 | A1274 | G1278 | G1279 | G1280 | G1281 | U1282 | G1283 | A1284  | G1285 | A1286 | A1287 | U1288 | G1289 | C1290  | G1291 | U1292 | G1295 | G1296 | C1297 | G1298 | G1299 | U1300 | A1301 | A1302 | G1303 | U1303 | U1303 | U1313 | C1314 | G1315 | U1316 | A1317 | G1318 | G1319 | G1320 | A1321 | U1326 | G1327 | C1328 | G1329 | C1330 | A1331 |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| U1188 | A1189 | G1190 | G1191 | G1192 | G1193 | G1195 | G1197 | U1199 | C1200 | G1201 | G1202 | G1203 | A1204 | U1205 | G1208 | G1209 | A1210 | U1211 | G1212 | A1213 | A1214  | G1215 | G1216 | C1217 | A1220 | G1221 | C1221A | G1222 | C1221 | G1223 | C1224 | G1225 | A1226 | G1227 | C1228 | G1229 | G1230 | G1231 | G1232 | C1233 | G1234 | G1235 | G1236 | U1237 | U1238 | G1239 | U1240 | A1241 | G1242 | G1243 | G1244 | U1248 | U1249 | C1252 | G1253 | U1254 | C1255 | A1256 | G1257 | C1258 |      |      |      |      |      |      |      |      |      |      |      |      |
| C1119 | G1120 | C1121 | G1122 | C1123 | C1124 | G1125 | G1126 | U1130 | G1131 | U1131 | A1132 | U1133 | C1135 | G1136 | G1137 | G1138 | U1139 | C1140 | U1141 | U1142 | A1142A | A1143 | G1144 | C1145 | C1146 | C1147 | A1148  | G1149 | C1150 | G1151 | C1152 | G1153 | G1154 | A1155 | U1159 | G1160 | C1161 | U1165 | C1166 | U1167 | G1168 | G1169 | G1170 | G1171 | A1173 | G1174 | U1175 | G1176 | A1177 | C1178 | C1179 | C1180 | C1181 | U1182 | A1183 | G1183 | C1187 |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| G1055 | G1056 | A1057 | G1058 | G1059 | U1060 | U1061 | G1062 | G1063 | G1064 | U1065 | U1066 | A1067 | G1068 | A1069 | A1070 | G1071 | G1072 | A1073 | G1074 | C1075 | G1076  | A1077 | U1078 | C1079 | A1084 | A1085 | A1086  | G1087 | C1088 | G1089 | U1090 | G1091 | C1092 | G1093 | U1094 | A1095 | A1096 | U1097 | A1098 | G1099 | G1100 | C1101 | G1102 | G1103 | C1104 | U1105 | G1106 | G1107 | U1108 | G1109 | G1110 | A1111 | G1112 | U1113 | A1114 | G1115 | C1116 | G1117 |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| G974  | C975  | A983  | G989  | C992  | G993  | C994  | C995  | A996  | G997  | C998  | U999  | A1000 | C1006 | A1009 | A1010 | G1011 | U1012 | C1013 | U1014 | G1015 | G1016  | U1019 | A1020 | A1021 | G1022 | U1023 | G1024  | U1025 | U1026 | A1027 | A1028 | A1029 | A953  | G954  | C955  | G956  | U958  | C959  | C960  | C961  | G962  | U963  | C964  | A965  | U966  | A1045 | U1046 | G1047 | A1048 | C1049 | A1050 | G1051 | A1054 |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| U907  | C908  | A909  | A910  | C914  | C915  | G916  | A917  | C918  | A918  | G921  | U922  | C923  | C924  | C925  | A926  | U930  | G931  | G932  | A933  | G934  | C935   | C936  | G940  | A941  | G942  | U943  | G944   | A945  | G946  | G947  | G948  | G952  | A953  | G954  | C955  | G956  | U958  | A959  | A960  | C961  | G962  | U963  | C964  | C965  | G966  | A1045 | U1046 | G1047 | A1048 | C1049 | A1050 | G1051 | A1054 |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| C840  | G843  | A844  | U847  | G848  | A849  | C850  | G852  | G853  | C856  | C857  | U858  | G859  | U860  | A861  | G862  | A863  | G864  | C865  | C866  | C867  | U868   | A869  | U870  | A871  | A872  | C876  | U877   | A878  | G879  | G880  | G881  | G882  | C883  | C884  | C885  | C886  | A887  | C888  | C889  | A890  | C892  | C893  | C894  | U895  | A896  | C897  | C898  | A899  | A900  | U901  | C902  | C903  | C904  | U905  |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| G770  | G771  | C772  | U773  | A774  | G775  | U776  | A777  | G778  | U779  | G780  | A781  | G782  | A783  | U784  | G785  | C786  | U787  | A788  | C789  | U790  | G791   | G792  | A793  | C795  | G796  | C797  | A802   | U803  | A804  | C732  | G733  | U734  | G738  | C739  | U740  | G741  | G742  | G743  | G744  | U747  | G748  | C749  | A752  | C753  | C754  | C755  | C756  | A761  | G763  | A764  | G769  |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| A643  | A644  | A645  | A646  | G647  | C650  | G651  | C652  | A653  | A654  | C655  | A656  | C657  | U658  | A659  | C659  | A660  | C661  | C662  | C663  | C664  | C665   | C666  | U657  | C658  | C659  | G660  | C661   | G662  | G663  | C664  | C665  | C666  | C672  | C673  | G674  | A675  | A676  | G680  | C683  | G682  | C683  | G686  | C687  | G688  | G689  | G690  | G691  | G692  | G693  | G694  | G695  | G696  | G697  | G698  | G699  | G700  | G701  | U702  | U703  | A706  | G707 | C708 | G709 | A752 | C753 | C754 | C755 | C756 | A761 | G763 | A764 | G769 |
| U688  | A689  | G690  | C691  | C692  | C693  | U694  | G695  | A696  | G697  | C698  | A699  | G700  | U701  | G702  | U703  | A706  | G707  | C708  | U709  | G710  | G711   | G712  | A793  | C795  | G796  | C797  | A802   | U803  | A804  | C732  | G733  | U734  | G738  | C739  | U740  | G741  | G742  | G743  | G744  | U747  | G748  | C749  | A752  | C753  | C754  | C755  | C756  | A761  | G763  | A764  | G769  |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| G491  | A492  | G493  | G494  | G500  | A501  | A502  | A505  | G508  | C509  | G512  | A518  | G519  | G522  | C523  | U524  | U525  | C526  | C527  | A528  | A529  | U530   | C531  | A532  | U533  | U534  | C535  | A536   | C537  | U538  | G381  | G382  | C385  | G386  | U387  | G388  | G389  | G396  | A402  | U403  | C404  | U405  | G406  | G407  | G408  | G409  | G410  | G411  | A412  | G413  | A414  | A415  |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| G418  | C419  | C420  | U421  | A422  | C423  | G424  | G425  | U427  | A428  | C433  | U434  | C435  | C436  | G437  | G438  | G440  | A443  | C444  | C445  | G446  | A447   | U448  | A449  | C451  | A454  | C455  | C456   | A457  | G458  | U459  | A460  | C461  | C462  | G463  | U464  | G465  | A466  | G467  | G468  | A469  | G470  | G473  | G476  | A477  | A478  | A479  | G480  | G481  | A482  | C483  | A484  |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |

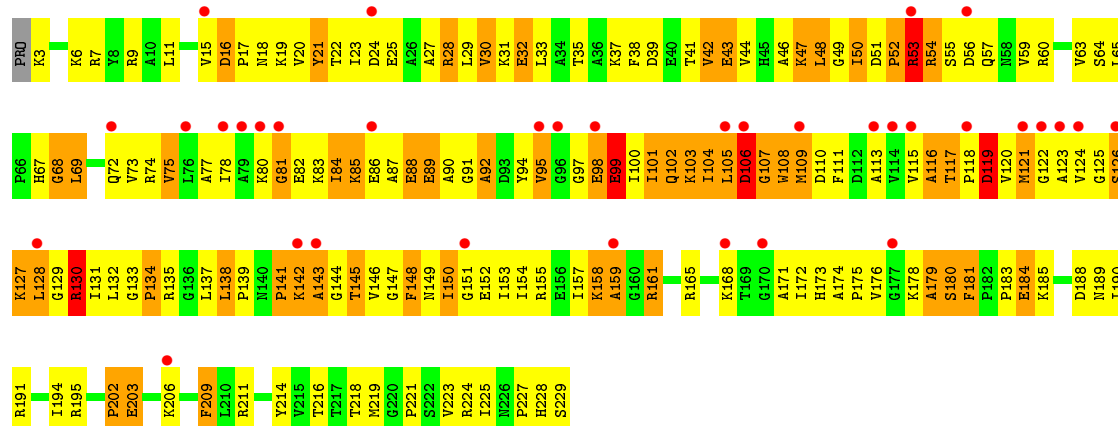
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| U2408 | C2343 | G2271 | G2194 | G2127 | C2043 | A1981 | A1901 | G1817 | G1748  | A1570  | G1487  | U1420  |
| G2409 | U2344 | U2272 | C2195 | C2128 | A2043 | C1982 | C1902 | U1818 | A1749  | A1571  | G1488  | G1421  |
| G2410 | G2345 | A2273 | C2196 | C2129 | A2051 | G1983 | G1903 | U1819 | G1750  | A1572  | U1489  | G1422  |
| A2411 | A2346 | A2274 | G2052 | U2130 | G2052 | G1984 | G1904 | U1820 | C1680  | A1490  | G1423  | G1424  |
| G2414 | C2347 | C2275 | A2198 | U2132 | C2055 | G1985 | G1905 | A1821 | G1662  | U1577  | C1493  | G1425  |
| G2415 | C2350 | G2276 | A2199 | U2133 | G2056 | G1987 | G1907 | G1822 | G1663  | C1578  | C1494  | G1426  |
| U2419 | G2351 | A2278 | C2200 | A2133 | G2056 | G1988 | A1912 | G1823 | C1669  | A1580  | A1495  | A1427  |
| G2420 | A2352 | G2279 | C2201 | A2135 | A2060 | G1989 | A1913 | G1824 | C1670  | G1581  | A1496  | C1428  |
| G2421 | G2353 | G2280 | U2203 | C2136 | A2061 | G1990 | C1914 | C1827 | G1763  | C1584  | G1429  | G1430  |
| G2422 | C2354 | C2205 | C2362 | U2137 | A2062 | U1991 | G1915 | G1828 | G1764  | A1586  | U1431  | U1432  |
| U2423 | C2355 | C2284 | G2206 | C2138 | G2065 | G1992 | G1916 | A1829 | U1766  | C1587  | U1433  | U1434  |
| U2424 | C2356 | C2285 | G2207 | U2139 | C2066 | G1993 | A1917 | G1835 | C1677  | C1588  | C1435  | C1436  |
| A2425 | U2357 | A2286 | A2208 | C2140 | G2067 | C1994 | A1918 | G1836 | U1768  | G1592  | G1437  | G1437  |
| A2426 | C2358 | A2287 | U2218 | G2141 | G2068 | U1995 | A1919 | C1837 | G1769  | G1593  | G1441  | G1442  |
| G2427 | G2359 | A2288 | G2219 | C2142 | U2074 | G1996 | C1920 | G1838 | G1770  | C1589  | A1509B | G1443  |
| G2428 | A2360 | G2291 | G2220 | U2143 | G2070 | G1997 | G1921 | G1845 | G1771  | C1590  | G1445  | G1446  |
| G2429 | A2361 | C2292 | G2221 | U2144 | A2071 | G1998 | G1922 | G1846 | U1772  | A1596  | A1445A | C1446A |
| A2430 | C2362 | C2293 | G2222 | C2145 | C2078 | C1999 | U1923 | G1847 | U1773  | C1598  | C1446  | G1447  |
| U2431 | C2363 | C2297 | G2223 | C2146 | U2079 | G2000 | C1924 | G1848 | A1774  | C1599  | G1448  | G1449  |
| A2432 | G2364 | A2298 | G2224 | G2147 | U2075 | A2001 | G1925 | G1849 | U1775  | C1599B | G1450  | G1451  |
| G2433 | G2365 | C2226 | U2076 | U2075 | G2087 | G2002 | U1926 | G1850 | G1776  | C1599C | G1452  | G1453  |
| A2439 | A2369 | G2230 | C2078 | U2078 | U2086 | C2006 | A1927 | G1851 | U1777  | C1599D | G1454  | G1455  |
| G2440 | G2370 | G2231 | U2079 | U2079 | G2087 | C2007 | G1930 | G1852 | U1778  | C1599E | G1456  | G1457  |
| C2441 | G2371 | C2232 | G2080 | U2080 | G2087 | C2008 | U1931 | G1853 | A1779  | C1599F | G1458  | G1459  |
| C2442 | G2372 | U2233 | U2081 | G2081 | G2088 | C2009 | A1932 | G1854 | A1780  | C1599G | G1460  | G1461  |
| G2443 | G2373 | G2234 | G2082 | G2082 | G2088 | G2010 | G1933 | G1855 | C1781  | C1599H | C1462  | C1463  |
| G2444 | A2376 | G2235 | G2083 | U2083 | G2090 | U2011 | A1936 | G1856 | C1782  | C1599I | C1464  | C1465  |
| G2445 | A2377 | G2236 | U2084 | U2084 | U2091 | G2012 | A1937 | G1857 | A1783  | C1599J | G1466  | G1467  |
| G2446 | A2378 | G2237 | U2085 | U2085 | U2092 | A2013 | A1938 | G1858 | G1784  | C1599K | G1468  | G1469  |
| G2447 | G2379 | G2238 | G2086 | U2086 | U2093 | A2014 | U1939 | G1859 | A1785  | C1599L | G1470  | G1471  |
| A2448 | C2380 | G2239 | C2087 | U2087 | U2094 | A2015 | C1941 | G1860 | G1786  | C1599M | G1472  | G1473  |
| U2449 | C2381 | G2240 | U2088 | U2088 | U2095 | U2016 | C1942 | G1861 | A1787  | C1599N | G1474  | G1475  |
| G2454 | G2382 | A2241 | C2089 | U2089 | U2096 | U2017 | G1945 | G1862 | A1788  | C1599O | G1476  | G1477  |
| U2457 | G2383 | A2242 | G2090 | U2090 | U2097 | G2018 | U1946 | G1863 | A1789  | C1599P | G1478  | G1479  |
| G2458 | C2384 | U2243 | U2091 | A2170 | U2098 | A2019 | U1947 | G1864 | U1790  | C1599Q | G1480  | G1481  |
| C2461 | C2385 | U2244 | G2100 | A2171 | U2099 | A2020 | G1948 | G1865 | G1702  | C1599R | G1482  | G1483  |
| U2462 | U2387 | U2245 | G2101 | U2172 | G2101 | C2021 | U1949 | G1866 | G1703  | C1599S | G1484  | G1485  |
| C2463 | A2388 | G2246 | U2102 | U2173 | U2102 | G2022 | G1954 | G1867 | U1709  | C1599T | G1486  | G1487  |
| C2464 | G2389 | A2247 | C2103 | C2175 | U2103 | G2023 | U1955 | G1868 | C1710  | C1599U | G1488  | G1489  |
| G2465 | U2390 | C2248 | G2104 | C2176 | G2104 | C2025 | U1956 | G1869 | C1711  | C1599V | G1490  | G1491  |
| C2466 | G2391 | U2249 | G2105 | C2177 | G2105 | C2026 | C1961 | G1870 | C1712  | C1599W | G1492  | G1493  |
| C2467 | A2392 | G2252 | U2109 | C2178 | G2106 | G2027 | U1962 | G1871 | U1713  | C1599X | G1494  | G1495  |
| G2468 | C2393 | G2253 | U2110 | U2180 | U2109 | G2028 | U1963 | G1872 | G1714  | C1599Y | G1496  | G1497  |
| A2469 | G2394 | U2257 | G2111 | G2181 | G2110 | A2030 | G1964 | G1873 | A1641  | C1599Z | G1498  | G1499  |
| G2470 | G2395 | U2258 | C2112 | G2182 | C2111 | A2031 | G1965 | G1874 | G1715  | C1599A | G1499  | G1500  |
| C2475 | U2396 | G2259 | G2113 | C2183 | G2112 | G2032 | A1966 | G1875 | G1716  | C1599B | G1501  | G1502  |
| A2476 | U2397 | G2260 | G2115 | G2184 | G2115 | A2033 | C1967 | G1876 | C1717  | C1599C | G1503  | G1504  |
| G2477 | G2398 | C2261 | C2185 | G2185 | G2116 | U2034 | G1968 | G1877 | G1718  | C1599D | C1505  | C1506  |
| A2478 | U2400 | U2262 | G2186 | G2186 | A2117 | G2035 | A1969 | G1878 | G1719  | C1599E | C1507  | C1508  |
| G2479 | C2402 | C2263 | G2187 | G2187 | U2118 | C2036 | A1970 | G1879 | C1720  | C1599F | C1509  | C1510  |
| C2480 | C2403 | G2264 | U2188 | G2188 | U2119 | G2037 | A1971 | G1880 | A1741  | C1599G | C1511  | C1512  |
| G2481 | C2404 | A2267 | U2189 | G2189 | G2123 | C2038 | A1972 | G1881 | C1745A | C1599H | C1513  | C1514  |
| U2482 | G2405 | A2268 | G2190 | G2190 | G2124 | C2039 | G1973 | G1882 | G1746  | C1599I | C1515  | C1516  |
| C2483 | U2406 | A2269 | G2191 | G2191 | G2125 | U2041 | C1974 | G1883 | G1747  | C1599J | C1517  | C1518  |
| G2484 | G2407 | G2270 | G2192 | G2193 | A2126 | A2042 | G1980 | G1884 | G1747A | C1599K | C1519  | C1520  |



• Molecule 36: 5S RIBOSOMAL RNA

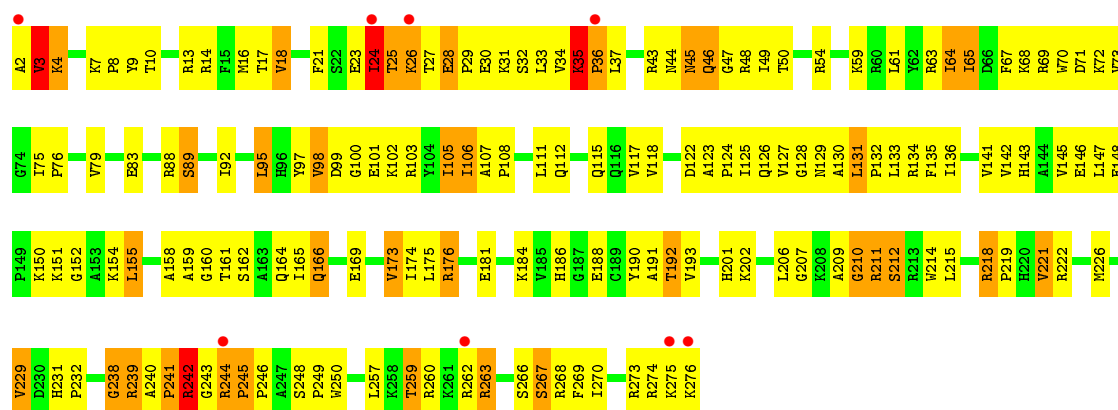


• Molecule 37: RIBOSOMAL PROTEIN L1

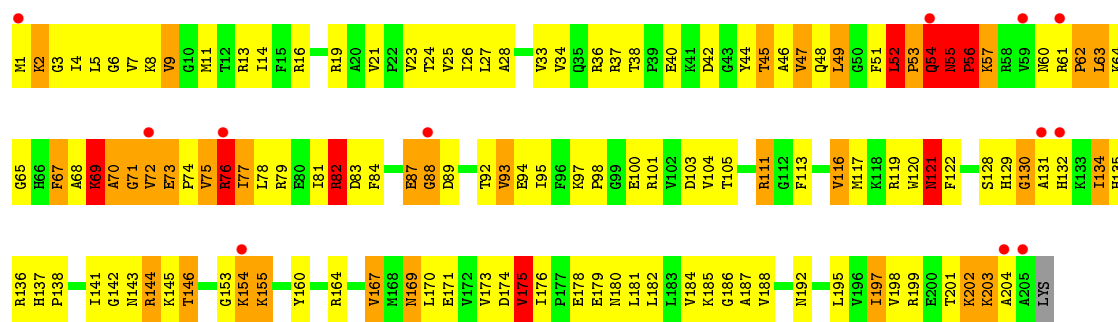


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

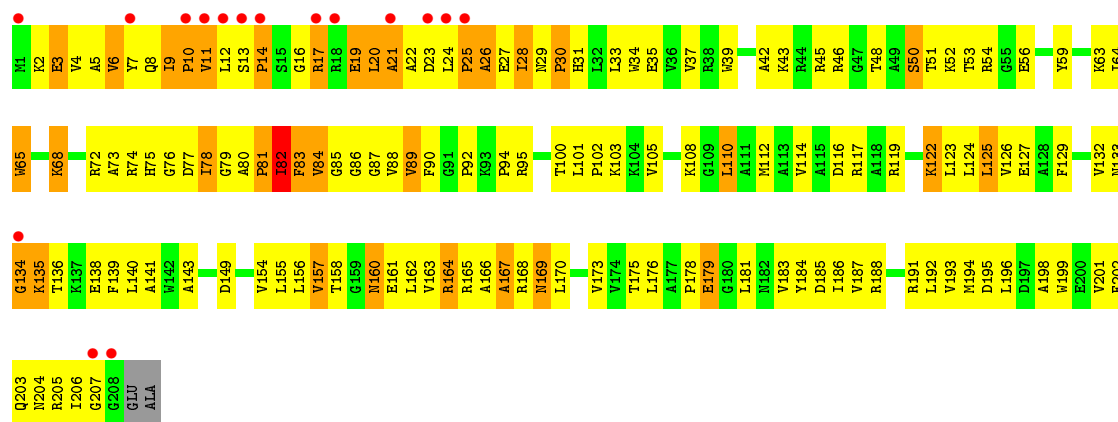




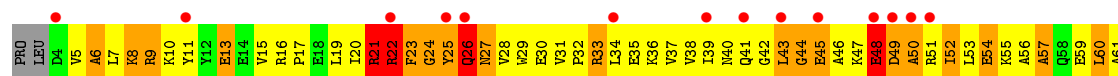
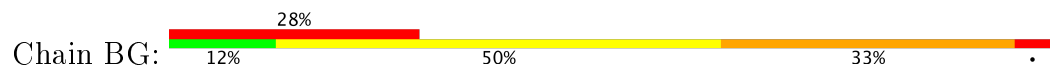
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

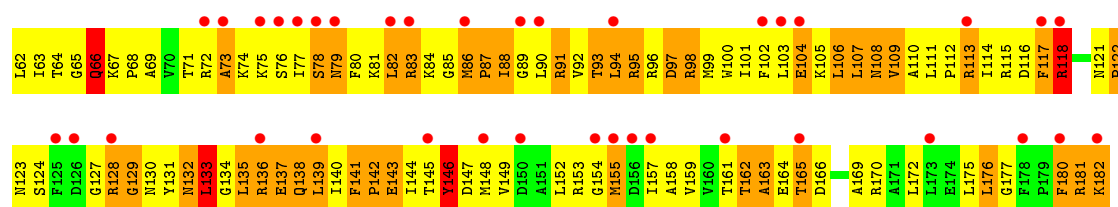


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

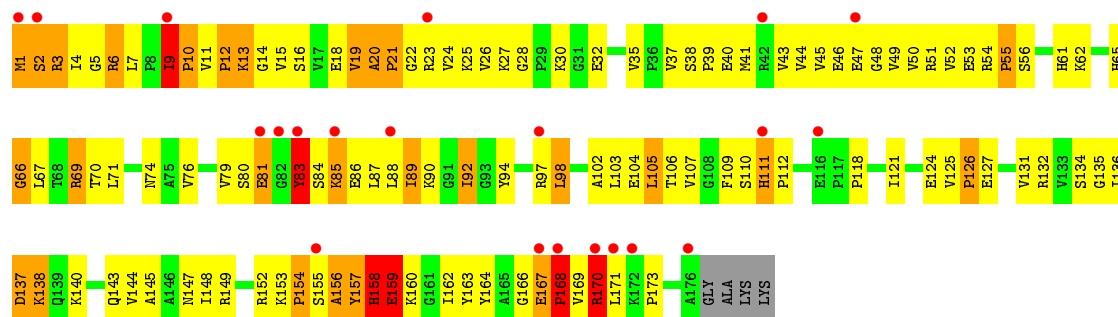


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

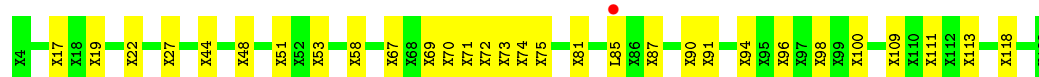
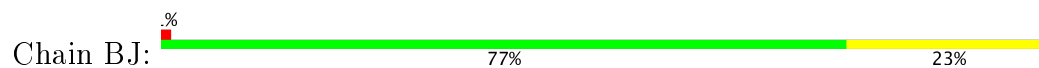




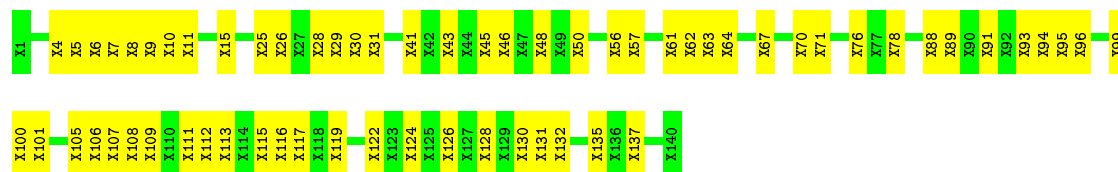
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



• Molecule 43: CHAIN J



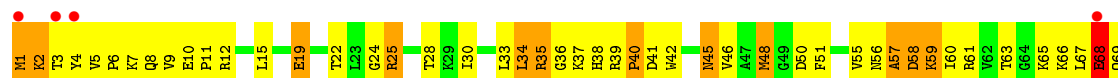
• Molecule 44: CHAIN K



• Molecule 45: CHAIN L



• Molecule 46: 50S RIBOSOMAL PROTEIN L13

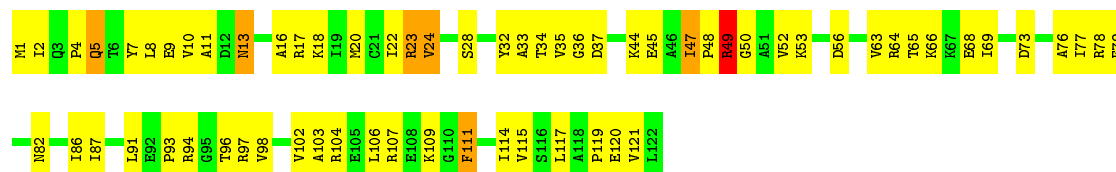






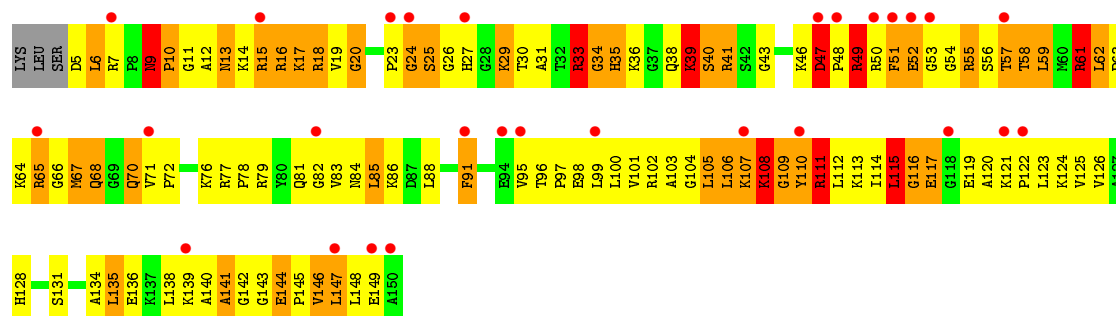
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 46% 48% 5% •



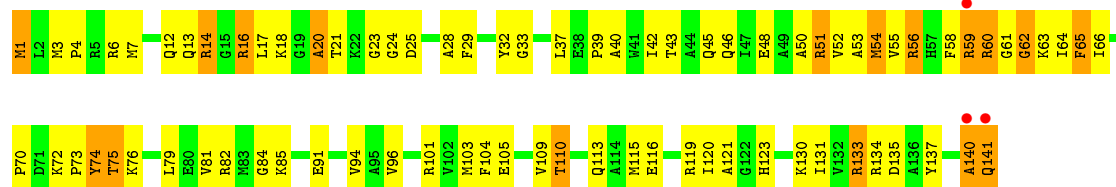
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 19% 46% 27% 6% •



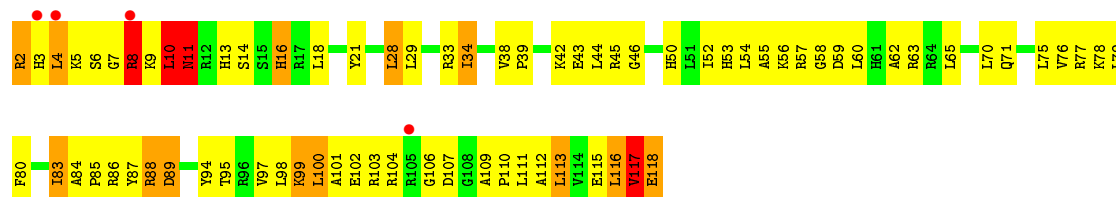
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ: 2% 44% 44% 12% •



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

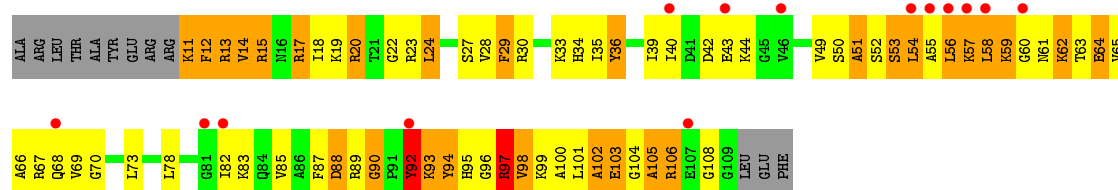
Chain BR: 3% 36% 50% 11% •



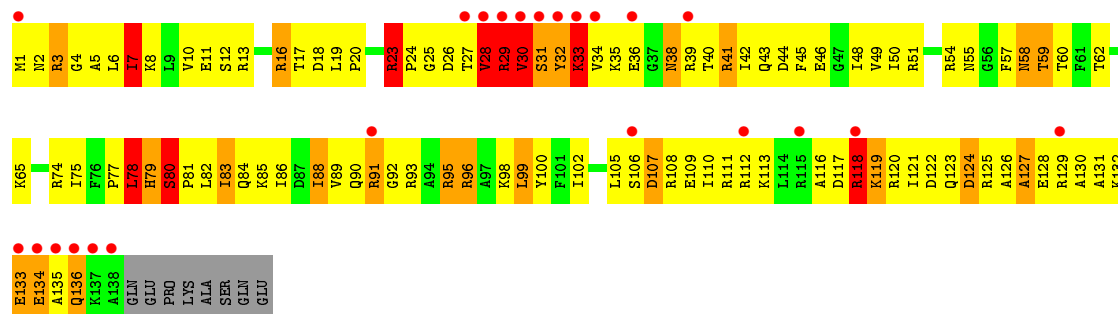
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS: 13% 24% 38% 25% 11% •

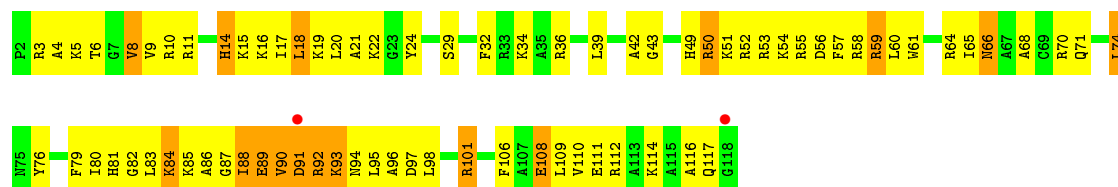




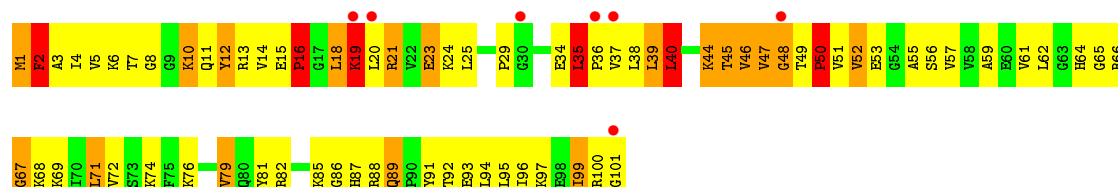
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



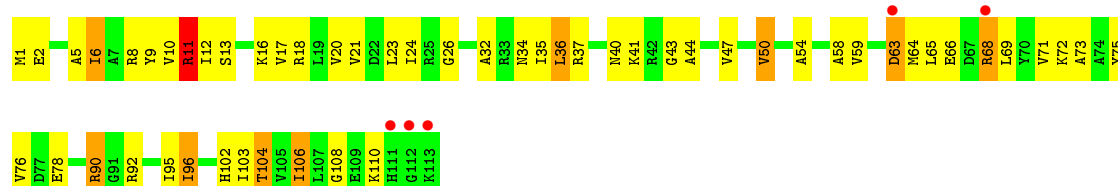
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



• Molecule 54: 50S RIBOSOMAL PROTEIN L21

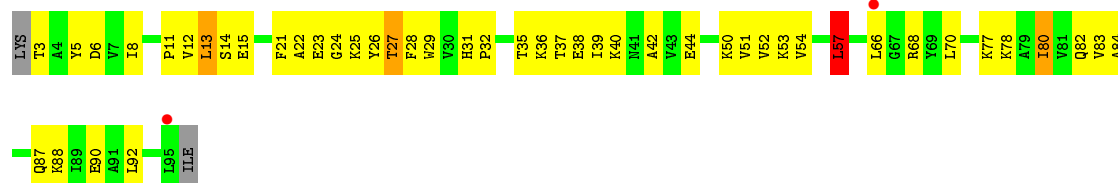


• Molecule 55: 50S RIBOSOMAL PROTEIN L22




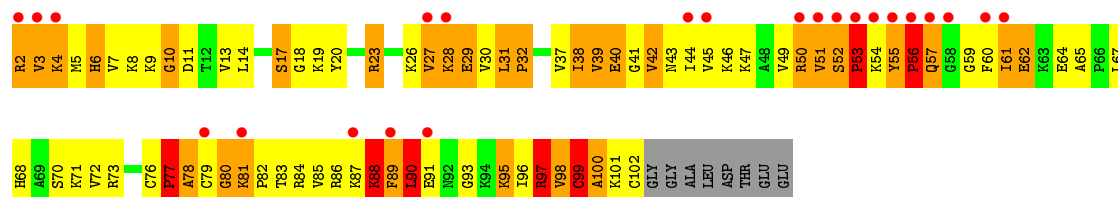
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX: 



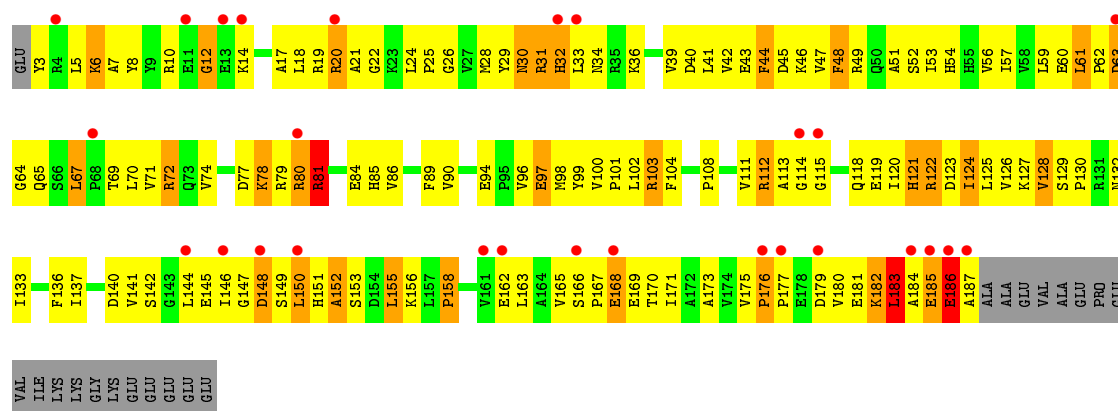
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY: 



- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ: 



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 202.90 Å   242.63 Å   309.32 Å<br>90.00°   99.60°   90.00°  | Depositor        |
| Resolution (Å)  | 49.75 – 2.95<br>49.75 – 2.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (49.75-2.95)<br>100.0 (49.75-2.95)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.26  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.70 (at 2.96 Å)  | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.210   ,   0.244<br>0.226   ,   0.256                      | Depositor<br>DCC |
| $R_{free}$ test set   | 30895 reflections (5.26%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.6  | Xtriage          |
| Anisotropy  | 0.435   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 60.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 153829  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 58.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: GCP, ZN, MG

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$    |
| 1   | AA    | 0.41         | 0/36258       | 0.70        | 5/56589 (0.0%) |
| 2   | AB    | 0.26         | 0/1936        | 0.46        | 0/2611         |
| 3   | AC    | 0.36         | 0/1637        | 0.58        | 0/2207         |
| 4   | AD    | 0.36         | 0/1733        | 0.61        | 0/2318         |
| 5   | AE    | 0.46         | 0/1163        | 0.67        | 0/1566         |
| 6   | AF    | 0.36         | 0/856         | 0.63        | 0/1154         |
| 7   | AG    | 0.36         | 0/1276        | 0.62        | 0/1709         |
| 8   | AH    | 0.39         | 0/1136        | 0.69        | 0/1527         |
| 9   | AI    | 0.36         | 0/1029        | 0.69        | 0/1379         |
| 10  | AJ    | 0.40         | 0/808         | 0.69        | 0/1087         |
| 11  | AK    | 0.39         | 0/900         | 0.68        | 0/1213         |
| 12  | AL    | 0.42         | 0/987         | 0.73        | 1/1322 (0.1%)  |
| 13  | AM    | 0.32         | 0/948         | 0.60        | 0/1272         |
| 14  | AN    | 0.41         | 0/501         | 0.77        | 0/664          |
| 15  | AO    | 0.37         | 0/745         | 0.62        | 0/992          |
| 16  | AP    | 0.40         | 0/717         | 0.71        | 0/965          |
| 17  | AQ    | 0.40         | 0/837         | 0.69        | 0/1119         |
| 18  | AR    | 0.38         | 0/579         | 0.60        | 0/768          |
| 19  | AS    | 0.37         | 0/706         | 0.64        | 0/950          |
| 20  | AT    | 0.39         | 0/765         | 0.76        | 0/1007         |
| 21  | AU    | 0.43         | 0/213         | 0.62        | 0/279          |
| 22  | AV    | 0.84         | 2/1809 (0.1%) | 1.27        | 7/2819 (0.2%)  |
| 23  | AX    | 1.26         | 2/210 (1.0%)  | 1.37        | 2/325 (0.6%)   |
| 24  | AY    | 0.33         | 0/5477        | 0.61        | 3/7415 (0.0%)  |
| 25  | B0    | 0.29         | 0/671         | 0.43        | 0/892          |
| 26  | B1    | 0.37         | 0/739         | 0.58        | 0/983          |
| 27  | B2    | 10.54        | 1/600 (0.2%)  | 0.42        | 0/793          |
| 28  | B3    | 0.32         | 0/473         | 0.50        | 0/636          |
| 29  | B4    | 0.29         | 0/594         | 0.45        | 0/795          |
| 30  | B5    | 0.40         | 0/473         | 0.70        | 0/639          |
| 31  | B6    | 0.48         | 0/440         | 0.80        | 0/586          |
| 32  | B7    | 0.44         | 0/427         | 0.71        | 0/561          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 33  | B8    | 0.56         | 0/516           | 0.87        | 1/681 (0.1%)     |
| 34  | B9    | 0.45         | 0/310           | 0.72        | 0/407            |
| 35  | BA    | 0.46         | 1/69972 (0.0%)  | 0.72        | 25/109230 (0.0%) |
| 36  | BB    | 0.37         | 0/2853          | 0.72        | 1/4451 (0.0%)    |
| 37  | BC    | 0.32         | 0/1766          | 0.62        | 0/2380           |
| 38  | BD    | 0.47         | 0/2195          | 0.82        | 1/2955 (0.0%)    |
| 39  | BE    | 0.42         | 0/1597          | 0.71        | 0/2155           |
| 40  | BF    | 0.39         | 0/1659          | 0.66        | 0/2246           |
| 41  | BG    | 0.45         | 0/1483          | 0.80        | 1/1994 (0.1%)    |
| 42  | BH    | 0.40         | 0/1371          | 0.67        | 0/1853           |
| 43  | BJ    | 0.20         | 0/7             | 0.87        | 0/8              |
| 46  | BN    | 0.46         | 0/1132          | 0.76        | 0/1527           |
| 47  | BO    | 0.44         | 0/943           | 0.71        | 0/1269           |
| 48  | BP    | 0.45         | 0/1131          | 0.86        | 4/1504 (0.3%)    |
| 49  | BQ    | 0.41         | 0/1143          | 0.65        | 0/1527           |
| 50  | BR    | 0.43         | 0/974           | 0.75        | 0/1302           |
| 51  | BS    | 0.39         | 0/779           | 0.66        | 0/1038           |
| 52  | BT    | 0.42         | 0/1156          | 0.66        | 0/1544           |
| 53  | BU    | 0.48         | 0/975           | 0.70        | 0/1297           |
| 54  | BV    | 0.40         | 0/790           | 0.72        | 0/1057           |
| 55  | BW    | 0.42         | 0/907           | 0.71        | 0/1216           |
| 56  | BX    | 0.47         | 0/740           | 0.69        | 1/995 (0.1%)     |
| 57  | BY    | 0.52         | 0/789           | 0.87        | 0/1053           |
| 58  | BZ    | 0.34         | 0/1500          | 0.63        | 0/2037           |
| All | All   | 0.77         | 6/164331 (0.0%) | 0.71        | 52/244868 (0.0%) |

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                   | 1                   |
| 24  | AY    | 0                   | 1                   |
| 35  | BA    | 0                   | 19                  |
| 36  | BB    | 0                   | 2                   |
| All | All   | 0                   | 23                  |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 27  | B2    | 72  | ALA  | C-OXT | 258.07 | 6.13        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 35  | BA    | 1453 | U    | O3'-P | -17.05 | 1.40        | 1.61     |
| 22  | AV    | 37   | A    | N3-C4 | 7.56   | 1.39        | 1.34     |
| 22  | AV    | 37   | A    | C6-N1 | 7.26   | 1.40        | 1.35     |
| 23  | AX    | 11   | A    | N9-C4 | 5.43   | 1.41        | 1.37     |
| 23  | AX    | 11   | A    | N3-C4 | 5.08   | 1.37        | 1.34     |

All (52) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 35  | BA    | 2208   | A    | P-O3'-C3'   | 9.92  | 131.60      | 119.70   |
| 22  | AV    | 37     | A    | N1-C2-N3    | -9.87 | 124.36      | 129.30   |
| 22  | AV    | 74     | C    | O4'-C1'-N1  | 8.40  | 114.92      | 108.20   |
| 22  | AV    | 37     | A    | N9-C4-C5    | -7.54 | 102.79      | 105.80   |
| 22  | AV    | 37     | A    | N1-C6-N6    | 6.87  | 122.72      | 118.60   |
| 23  | AX    | 18     | C    | N1-C2-O2    | -6.77 | 114.84      | 118.90   |
| 1   | AA    | 189(H) | G    | N9-C1'-C2'  | -6.57 | 104.77      | 112.00   |
| 22  | AV    | 37     | A    | C8-N9-C4    | 6.50  | 108.40      | 105.80   |
| 22  | AV    | 37     | A    | C2-N3-C4    | 6.30  | 113.75      | 110.60   |
| 23  | AX    | 13     | A    | C2-N3-C4    | -6.26 | 107.47      | 110.60   |
| 35  | BA    | 1453   | U    | OP2-P-O3'   | 6.15  | 118.74      | 105.20   |
| 35  | BA    | 945    | A    | N9-C1'-C2'  | 5.99  | 121.78      | 114.00   |
| 38  | BD    | 210    | GLY  | N-CA-C      | -5.97 | 98.17       | 113.10   |
| 35  | BA    | 387    | U    | C2'-C3'-O3' | 5.91  | 123.15      | 113.70   |
| 48  | BP    | 41     | ARG  | N-CA-C      | -5.91 | 95.05       | 111.00   |
| 41  | BG    | 22     | ARG  | N-CA-C      | -5.87 | 95.15       | 111.00   |
| 35  | BA    | 1495   | A    | N9-C1'-C2'  | 5.79  | 121.53      | 114.00   |
| 24  | AY    | 356    | LEU  | CA-CB-CG    | 5.78  | 128.59      | 115.30   |
| 56  | BX    | 57     | LEU  | CA-CB-CG    | 5.68  | 128.36      | 115.30   |
| 35  | BA    | 2481   | G    | N9-C1'-C2'  | 5.65  | 121.35      | 114.00   |
| 1   | AA    | 428    | G    | C2'-C3'-O3' | 5.63  | 122.71      | 113.70   |
| 35  | BA    | 2136   | C    | C2'-C3'-O3' | 5.60  | 122.66      | 113.70   |
| 48  | BP    | 24     | GLY  | N-CA-C      | 5.55  | 126.98      | 113.10   |
| 24  | AY    | 260    | LEU  | CA-CB-CG    | 5.53  | 128.02      | 115.30   |
| 48  | BP    | 20     | GLY  | N-CA-C      | -5.51 | 99.34       | 113.10   |
| 35  | BA    | 783    | A    | N9-C1'-C2'  | -5.50 | 105.95      | 112.00   |
| 35  | BA    | 2542   | A    | N9-C1'-C2'  | 5.42  | 121.04      | 114.00   |
| 33  | B8    | 32     | LEU  | CA-CB-CG    | 5.34  | 127.58      | 115.30   |
| 35  | BA    | 310    | A    | C5'-C4'-C3' | -5.33 | 107.48      | 116.00   |
| 35  | BA    | 1015   | G    | C5'-C4'-C3' | -5.32 | 107.49      | 116.00   |
| 35  | BA    | 512    | G    | O4'-C1'-N9  | 5.29  | 112.43      | 108.20   |
| 22  | AV    | 18     | G    | N3-C4-C5    | -5.27 | 125.97      | 128.60   |
| 35  | BA    | 1159   | U    | C5'-C4'-C3' | -5.26 | 107.58      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BA    | 708  | C    | C5'-C4'-C3' | -5.25 | 107.60      | 116.00   |
| 35  | BA    | 1947 | C    | C5'-C4'-C3' | -5.24 | 107.61      | 116.00   |
| 1   | AA    | 1117 | G    | C5'-C4'-O4' | -5.23 | 102.82      | 109.10   |
| 48  | BP    | 29   | LYS  | N-CA-C      | -5.18 | 97.01       | 111.00   |
| 35  | BA    | 1493 | C    | N1-C1'-C2'  | 5.17  | 120.73      | 114.00   |
| 35  | BA    | 1558 | A    | C2'-C3'-O3' | 5.17  | 121.97      | 113.70   |
| 36  | BB    | 44   | G    | N9-C1'-C2'  | 5.15  | 120.70      | 114.00   |
| 1   | AA    | 243  | A    | N9-C1'-C2'  | 5.15  | 120.69      | 114.00   |
| 35  | BA    | 74   | A    | C2'-C3'-O3' | 5.15  | 121.94      | 113.70   |
| 35  | BA    | 2665 | A    | N9-C1'-C2'  | -5.13 | 106.35      | 112.00   |
| 12  | AL    | 26   | ALA  | N-CA-C      | -5.12 | 97.17       | 111.00   |
| 24  | AY    | 379  | GLY  | N-CA-C      | -5.11 | 100.32      | 113.10   |
| 35  | BA    | 1549 | C    | C5'-C4'-C3' | -5.11 | 107.82      | 116.00   |
| 35  | BA    | 2346 | A    | O4'-C1'-N9  | 5.11  | 112.29      | 108.20   |
| 35  | BA    | 2346 | A    | N9-C1'-C2'  | 5.08  | 120.61      | 114.00   |
| 35  | BA    | 1838 | C    | N1-C1'-C2'  | 5.08  | 120.61      | 114.00   |
| 1   | AA    | 1054 | C    | C5'-C4'-C3' | -5.07 | 107.88      | 116.00   |
| 35  | BA    | 2581 | G    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 35  | BA    | 2286 | A    | N9-C1'-C2'  | 5.02  | 120.52      | 114.00   |

There are no chirality outliers.

All (23) planarity outliers are listed below:

| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 1   | AA    | 189(H) | G    | Sidechain |
| 24  | AY    | 499    | ARG  | Sidechain |
| 35  | BA    | 1192   | G    | Sidechain |
| 35  | BA    | 2414   | G    | Sidechain |
| 35  | BA    | 2464   | C    | Sidechain |
| 35  | BA    | 2504   | U    | Sidechain |
| 35  | BA    | 2508   | G    | Sidechain |
| 35  | BA    | 2516   | G    | Sidechain |
| 35  | BA    | 2542   | A    | Sidechain |
| 35  | BA    | 2578   | G    | Sidechain |
| 35  | BA    | 2581   | G    | Sidechain |
| 35  | BA    | 2595   | G    | Sidechain |
| 35  | BA    | 2597   | G    | Sidechain |
| 35  | BA    | 2664   | G    | Sidechain |
| 35  | BA    | 271(H) | G    | Sidechain |
| 35  | BA    | 271(Q) | G    | Sidechain |
| 35  | BA    | 271(Y) | U    | Sidechain |
| 35  | BA    | 2746   | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BA    | 2779 | U    | Sidechain |
| 35  | BA    | 2848 | G    | Sidechain |
| 35  | BA    | 476  | G    | Sidechain |
| 36  | BB    | 16   | G    | Sidechain |
| 36  | BB    | 67   | G    | 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    | 32391 | 0        | 16349    | 1994    | 0            |
| 2   | AB    | 1901  | 0        | 1947     | 322     | 1            |
| 3   | AC    | 1613  | 0        | 1677     | 223     | 28           |
| 4   | AD    | 1703  | 0        | 1765     | 125     | 0            |
| 5   | AE    | 1147  | 0        | 1207     | 56      | 0            |
| 6   | AF    | 843   | 0        | 857      | 53      | 0            |
| 7   | AG    | 1257  | 0        | 1296     | 138     | 0            |
| 8   | AH    | 1116  | 0        | 1177     | 63      | 0            |
| 9   | AI    | 1010  | 0        | 1037     | 150     | 0            |
| 10  | AJ    | 795   | 0        | 840      | 114     | 0            |
| 11  | AK    | 885   | 0        | 904      | 56      | 0            |
| 12  | AL    | 971   | 0        | 1057     | 112     | 0            |
| 13  | AM    | 938   | 0        | 995      | 124     | 0            |
| 14  | AN    | 492   | 0        | 529      | 68      | 0            |
| 15  | AO    | 734   | 0        | 771      | 49      | 0            |
| 16  | AP    | 701   | 0        | 720      | 58      | 0            |
| 17  | AQ    | 824   | 0        | 891      | 47      | 0            |
| 18  | AR    | 574   | 0        | 644      | 26      | 0            |
| 19  | AS    | 692   | 0        | 714      | 109     | 0            |
| 20  | AT    | 763   | 0        | 861      | 71      | 11           |
| 21  | AU    | 209   | 0        | 221      | 12      | 0            |
| 22  | AV    | 1619  | 0        | 823      | 58      | 0            |
| 23  | AX    | 188   | 0        | 98       | 7       | 0            |
| 24  | AY    | 5376  | 0        | 5433     | 565     | 0            |
| 25  | B0    | 662   | 0        | 688      | 160     | 0            |
| 26  | B1    | 732   | 0        | 808      | 114     | 0            |
| 27  | B2    | 598   | 0        | 651      | 125     | 11           |
| 28  | B3    | 468   | 0        | 523      | 66      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | B4    | 581   | 0        | 577      | 214     | 0            |
| 30  | B5    | 459   | 0        | 478      | 75      | 0            |
| 31  | B6    | 433   | 0        | 461      | 128     | 0            |
| 32  | B7    | 419   | 0        | 467      | 29      | 0            |
| 33  | B8    | 508   | 0        | 576      | 112     | 0            |
| 34  | B9    | 307   | 0        | 335      | 31      | 0            |
| 35  | BA    | 62476 | 0        | 31499    | 3288    | 28           |
| 36  | BB    | 2551  | 0        | 1295     | 107     | 0            |
| 37  | BC    | 1735  | 0        | 1790     | 277     | 1            |
| 38  | BD    | 2145  | 0        | 2234     | 255     | 0            |
| 39  | BE    | 1564  | 0        | 1629     | 233     | 0            |
| 40  | BF    | 1624  | 0        | 1677     | 220     | 0            |
| 41  | BG    | 1459  | 0        | 1516     | 395     | 0            |
| 42  | BH    | 1345  | 0        | 1430     | 187     | 0            |
| 43  | BJ    | 654   | 0        | 156      | 22      | 0            |
| 44  | BK    | 701   | 0        | 168      | 46      | 0            |
| 45  | BL    | 356   | 0        | 86       | 20      | 0            |
| 46  | BN    | 1105  | 0        | 1180     | 111     | 0            |
| 47  | BO    | 933   | 0        | 996      | 67      | 0            |
| 48  | BP    | 1114  | 0        | 1186     | 302     | 0            |
| 49  | BQ    | 1122  | 0        | 1179     | 111     | 0            |
| 50  | BR    | 960   | 0        | 1021     | 104     | 0            |
| 51  | BS    | 771   | 0        | 832      | 158     | 0            |
| 52  | BT    | 1142  | 0        | 1200     | 229     | 0            |
| 53  | BU    | 958   | 0        | 1015     | 122     | 0            |
| 54  | BV    | 779   | 0        | 852      | 147     | 0            |
| 55  | BW    | 896   | 0        | 953      | 56      | 0            |
| 56  | BX    | 726   | 0        | 778      | 47      | 0            |
| 57  | BY    | 776   | 0        | 870      | 164     | 0            |
| 58  | BZ    | 1468  | 0        | 1492     | 216     | 0            |
| 59  | AA    | 198   | 0        | 0        | 0       | 0            |
| 59  | AY    | 1     | 0        | 0        | 0       | 0            |
| 59  | B0    | 1     | 0        | 0        | 0       | 0            |
| 59  | B5    | 1     | 0        | 0        | 0       | 0            |
| 59  | BA    | 320   | 0        | 0        | 0       | 0            |
| 59  | BC    | 1     | 0        | 0        | 0       | 0            |
| 59  | BU    | 1     | 0        | 0        | 0       | 0            |
| 60  | AD    | 1     | 0        | 0        | 0       | 0            |
| 60  | AN    | 1     | 0        | 0        | 0       | 0            |
| 60  | B9    | 1     | 0        | 0        | 0       | 0            |
| 61  | AY    | 32    | 0        | 14       | 11      | 0            |
| 62  | AY    | 2     | 0        | 0        | 2       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| All | All   | 153829 | 0        | 105425   | 11645   | 40           |

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 45.

All (11645) 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:B5:46:CYS:SG    | 30:B5:47:PRO:HD2  | 1.41                     | 1.57              |
| 29:B4:12:ALA:H     | 29:B4:24:THR:CG2  | 1.16                     | 1.56              |
| 9:AI:19:LEU:HA     | 9:AI:61:ALA:CB    | 1.39                     | 1.53              |
| 52:BT:80:SER:HB3   | 52:BT:81:PRO:CD   | 1.40                     | 1.51              |
| 9:AI:18:PHE:C      | 9:AI:61:ALA:HB1   | 1.27                     | 1.50              |
| 42:BH:1:MET:SD     | 42:BH:1:MET:CE    | 2.04                     | 1.46              |
| 1:AA:311:C:C2'     | 1:AA:312:C:H5'    | 1.46                     | 1.45              |
| 1:AA:950:U:C2'     | 1:AA:951:G:H5''   | 1.41                     | 1.45              |
| 29:B4:12:ALA:N     | 29:B4:24:THR:CG2  | 1.79                     | 1.41              |
| 9:AI:19:LEU:CB     | 9:AI:61:ALA:HB2   | 1.48                     | 1.40              |
| 9:AI:19:LEU:CA     | 9:AI:61:ALA:HB2   | 0.93                     | 1.39              |
| 1:AA:950:U:H2'     | 1:AA:951:G:C5'    | 1.51                     | 1.39              |
| 35:BA:111:A:C2'    | 35:BA:112:U:H5'   | 1.51                     | 1.38              |
| 48:BP:84:ASN:CG    | 48:BP:116:GLY:HA3 | 1.45                     | 1.38              |
| 35:BA:967:C:C2'    | 35:BA:968:G:H5'   | 1.53                     | 1.37              |
| 35:BA:2555:U:C2'   | 35:BA:2556:C:H5'  | 1.56                     | 1.36              |
| 29:B4:12:ALA:N     | 29:B4:24:THR:HG21 | 1.38                     | 1.36              |
| 35:BA:252:G:OP2    | 48:BP:50:ARG:NH1  | 1.58                     | 1.35              |
| 37:BC:117:THR:HG22 | 37:BC:118:PRO:C   | 1.45                     | 1.33              |
| 27:B2:16:LEU:HD22  | 27:B2:20:GLU:CG   | 1.58                     | 1.33              |
| 48:BP:85:LEU:CD2   | 48:BP:117:GLU:O   | 1.76                     | 1.33              |
| 35:BA:954:G:C2'    | 35:BA:955:C:H5'   | 1.62                     | 1.29              |
| 1:AA:37:U:C2'      | 1:AA:38:G:H5'     | 1.63                     | 1.28              |
| 35:BA:1988:C:C2'   | 35:BA:1989:G:H5'  | 1.61                     | 1.28              |
| 29:B4:12:ALA:CA    | 29:B4:24:THR:HG21 | 1.63                     | 1.28              |
| 49:BQ:60:ARG:HG3   | 58:BZ:179:ASP:OD1 | 1.16                     | 1.28              |
| 9:AI:26:VAL:HG21   | 9:AI:61:ALA:O     | 1.32                     | 1.28              |
| 1:AA:545:C:C2'     | 1:AA:546:G:H5'    | 1.62                     | 1.27              |
| 35:BA:108:U:O2'    | 35:BA:109:G:H5'   | 1.35                     | 1.27              |
| 2:AB:228:GLY:CA    | 2:AB:229:VAL:HG22 | 1.65                     | 1.27              |
| 31:B6:7:ILE:HG21   | 31:B6:27:LYS:NZ   | 1.50                     | 1.26              |
| 35:BA:955:C:C2'    | 35:BA:956:G:H5'   | 1.66                     | 1.26              |
| 35:BA:1417:C:O2'   | 35:BA:1418:G:H5'  | 1.34                     | 1.26              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:AB:167:PRO:CD  | 2:AB:188:ALA:HB2  | 1.65                     | 1.26              |
| 35:BA:653:A:H5'  | 35:BA:654:A:OP2   | 1.35                     | 1.25              |
| 2:AB:89:GLY:O    | 2:AB:90:MET:HG2   | 1.35                     | 1.25              |
| 35:BA:1678:G:N2  | 35:BA:1989:G:H22  | 1.30                     | 1.25              |
| 1:AA:773:G:O2'   | 1:AA:774:G:H5'    | 1.33                     | 1.25              |
| 35:BA:1596:A:C2' | 35:BA:1597:A:H5'  | 1.64                     | 1.25              |
| 35:BA:246:C:C2'  | 35:BA:247:G:H5'   | 1.67                     | 1.25              |
| 1:AA:936:C:O2'   | 1:AA:937:A:H5'    | 1.36                     | 1.24              |
| 35:BA:697:C:O2'  | 35:BA:698:C:H5'   | 1.37                     | 1.24              |
| 35:BA:856:C:H2'  | 35:BA:857:C:C6    | 1.70                     | 1.24              |
| 29:B4:12:ALA:C   | 29:B4:24:THR:HG21 | 1.57                     | 1.24              |
| 1:AA:1371:G:C2'  | 1:AA:1372:U:H5'   | 1.68                     | 1.24              |
| 1:AA:775:G:O2'   | 1:AA:776:G:H5'    | 1.36                     | 1.24              |
| 35:BA:179:G:C2'  | 35:BA:180:G:H5'   | 1.66                     | 1.24              |
| 35:BA:953:A:C2'  | 35:BA:954:G:H5'   | 1.67                     | 1.24              |
| 1:AA:106:C:O2'   | 1:AA:107:G:H5'    | 1.34                     | 1.23              |
| 1:AA:590:C:O2'   | 1:AA:591:U:H5'    | 1.35                     | 1.23              |
| 35:BA:702:G:O2'  | 35:BA:703:U:H5'   | 1.37                     | 1.23              |
| 2:AB:231:GLU:HB2 | 2:AB:232:PRO:CD   | 1.67                     | 1.23              |
| 28:B3:9:VAL:HG11 | 28:B3:55:ARG:CD   | 1.69                     | 1.23              |
| 22:AV:41:C:O2'   | 22:AV:42:C:H5'    | 1.38                     | 1.23              |
| 1:AA:949:A:H2'   | 1:AA:950:U:C5'    | 1.67                     | 1.22              |
| 29:B4:12:ALA:C   | 29:B4:24:THR:CG2  | 2.06                     | 1.22              |
| 1:AA:266:G:C5'   | 1:AA:267:C:H5     | 1.52                     | 1.22              |
| 1:AA:543:C:C2'   | 1:AA:544:G:H5'    | 1.68                     | 1.22              |
| 1:AA:593:G:O2'   | 1:AA:594:G:H5'    | 1.36                     | 1.22              |
| 1:AA:770:C:O2'   | 1:AA:771:G:H5'    | 1.40                     | 1.22              |
| 2:AB:145:LEU:O   | 2:AB:149:LEU:HB2  | 1.39                     | 1.22              |
| 2:AB:228:GLY:HA2 | 2:AB:229:VAL:CG1  | 1.68                     | 1.21              |
| 35:BA:1773:A:C2' | 35:BA:1774:C:H5'  | 1.69                     | 1.21              |
| 35:BA:523:C:O2'  | 35:BA:524:U:H5'   | 1.37                     | 1.21              |
| 48:BP:47:ASP:HB3 | 48:BP:48:PRO:CA   | 1.71                     | 1.21              |
| 1:AA:490:G:O2'   | 1:AA:491:G:H5'    | 1.41                     | 1.21              |
| 1:AA:688:G:O2'   | 1:AA:689:C:H5'    | 1.38                     | 1.21              |
| 35:BA:2007:C:O2' | 35:BA:2008:C:H5'  | 1.41                     | 1.21              |
| 31:B6:10:LEU:CD2 | 31:B6:10:LEU:H    | 1.54                     | 1.21              |
| 35:BA:1902:C:O2' | 38:BD:244:ARG:HB2 | 1.40                     | 1.21              |
| 27:B2:16:LEU:CD2 | 27:B2:20:GLU:HG2  | 1.71                     | 1.21              |
| 1:AA:359:U:O2'   | 1:AA:360:A:H5'    | 1.36                     | 1.21              |
| 35:BA:1822:G:O2' | 35:BA:1823:G:H5'  | 1.37                     | 1.21              |
| 1:AA:360:A:O2'   | 1:AA:361:G:H5'    | 1.37                     | 1.20              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BA:1984:G:O2'  | 35:BA:1985:G:H5'  | 1.41                     | 1.20              |
| 9:AI:18:PHE:O     | 9:AI:61:ALA:HB1   | 1.08                     | 1.20              |
| 35:BA:2753:A:O2'  | 35:BA:2754:U:H5'  | 1.36                     | 1.20              |
| 35:BA:968:G:O2'   | 35:BA:969:U:H5'   | 1.40                     | 1.20              |
| 2:AB:187:LEU:HD23 | 2:AB:201:ILE:O    | 1.38                     | 1.20              |
| 1:AA:685:G:O2'    | 1:AA:686:U:H5'    | 1.40                     | 1.20              |
| 35:BA:1423:G:O2'  | 35:BA:1424:G:H5'  | 1.36                     | 1.19              |
| 35:BA:1464:C:O2'  | 35:BA:1465:G:H5'  | 1.42                     | 1.19              |
| 35:BA:179:G:H2'   | 35:BA:180:G:H5'   | 1.24                     | 1.19              |
| 1:AA:509:A:H5'    | 4:AD:54:TYR:CD2   | 1.76                     | 1.19              |
| 35:BA:2555:U:H2'  | 35:BA:2556:C:C5'  | 1.72                     | 1.19              |
| 3:AC:81:GLY:O     | 3:AC:82:GLU:HG3   | 1.42                     | 1.19              |
| 35:BA:2606:C:C2'  | 35:BA:2607:G:H5'  | 1.72                     | 1.19              |
| 35:BA:1720:U:H2'  | 35:BA:1721:G:H5'' | 1.25                     | 1.18              |
| 48:BP:51:PHE:CE2  | 48:BP:53:GLY:HA2  | 1.78                     | 1.18              |
| 1:AA:495:A:H4'    | 1:AA:496:A:H5'    | 1.26                     | 1.18              |
| 26:B1:29:GLY:HA3  | 35:BA:2396:G:O2'  | 1.41                     | 1.18              |
| 35:BA:1301:A:O2'  | 35:BA:1302:A:H2'  | 1.40                     | 1.18              |
| 35:BA:2715:C:O2'  | 35:BA:2716:U:H5'  | 1.43                     | 1.18              |
| 35:BA:39:C:O2'    | 35:BA:40:C:H5'    | 1.43                     | 1.18              |
| 35:BA:747:U:C2    | 35:BA:2613:U:O4   | 1.95                     | 1.18              |
| 57:BY:76:CYS:SG   | 57:BY:77:PRO:HD2  | 1.83                     | 1.18              |
| 35:BA:49:A:H5''   | 35:BA:51:G:O4'    | 1.44                     | 1.18              |
| 35:BA:605:C:O2'   | 35:BA:606:U:H5'   | 1.39                     | 1.18              |
| 57:BY:28:LYS:HD2  | 57:BY:28:LYS:H    | 1.06                     | 1.18              |
| 48:BP:84:ASN:ND2  | 48:BP:116:GLY:HA3 | 1.57                     | 1.17              |
| 1:AA:265:G:H2'    | 1:AA:266:G:H5''   | 1.26                     | 1.17              |
| 2:AB:14:GLY:O     | 2:AB:15:VAL:HG23  | 1.43                     | 1.17              |
| 2:AB:228:GLY:CA   | 2:AB:229:VAL:HG13 | 1.75                     | 1.17              |
| 37:BC:117:THR:CG2 | 37:BC:119:ASP:HB2 | 1.75                     | 1.17              |
| 35:BA:246:C:H2'   | 35:BA:247:G:C5'   | 1.73                     | 1.17              |
| 1:AA:556:C:O2'    | 1:AA:557:G:H5'    | 1.43                     | 1.17              |
| 35:BA:1222:C:O2'  | 35:BA:1223:G:H5'  | 1.45                     | 1.17              |
| 1:AA:862:C:C2'    | 1:AA:863:U:H5'    | 1.74                     | 1.17              |
| 35:BA:1778:U:O2'  | 35:BA:1779:U:H5'  | 1.40                     | 1.17              |
| 1:AA:774:G:O2'    | 1:AA:775:G:H5'    | 1.40                     | 1.17              |
| 30:B5:4:HIS:HB3   | 30:B5:5:PRO:HD3   | 1.23                     | 1.16              |
| 35:BA:1999:C:O2'  | 35:BA:2000:G:H5'  | 1.43                     | 1.16              |
| 27:B2:38:GLN:O    | 27:B2:41:ILE:HG13 | 1.43                     | 1.16              |
| 48:BP:57:THR:O    | 48:BP:59:LEU:N    | 1.78                     | 1.16              |
| 1:AA:119:A:O2'    | 1:AA:120:A:OP2    | 1.60                     | 1.16              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 9:AI:18:PHE:C       | 9:AI:61:ALA:CB     | 2.07                     | 1.16              |
| 35:BA:2201:C:O2'    | 35:BA:2202:C:H5'   | 1.43                     | 1.16              |
| 1:AA:687:A:H1'      | 1:AA:688:G:OP2     | 1.46                     | 1.16              |
| 7:AG:121:ALA:H      | 7:AG:124:LEU:HD13  | 1.09                     | 1.16              |
| 1:AA:37:U:H2'       | 1:AA:38:G:H5'      | 1.21                     | 1.15              |
| 1:AA:556:C:C2'      | 1:AA:557:G:H5'     | 1.75                     | 1.15              |
| 35:BA:1747(A):G:H2' | 35:BA:1748:G:H5''  | 1.25                     | 1.15              |
| 1:AA:1502:A:H2      | 1:AA:1505:G:N2     | 1.43                     | 1.15              |
| 35:BA:259:G:O2'     | 35:BA:260:G:H5'    | 1.43                     | 1.15              |
| 35:BA:2010:G:O2'    | 35:BA:2011:U:H5'   | 1.47                     | 1.15              |
| 35:BA:1137:G:O2'    | 35:BA:1138:G:H5'   | 1.46                     | 1.15              |
| 37:BC:80:LYS:HE3    | 37:BC:120:VAL:HG12 | 1.23                     | 1.15              |
| 13:AM:11:ARG:HA     | 13:AM:45:VAL:HB    | 1.25                     | 1.15              |
| 35:BA:1678:G:N2     | 35:BA:1989:G:N2    | 1.95                     | 1.15              |
| 40:BF:6:VAL:HG12    | 40:BF:7:TYR:H      | 1.12                     | 1.15              |
| 30:B5:51:TYR:O      | 30:B5:53:ALA:N     | 1.80                     | 1.15              |
| 1:AA:1179:A:O2'     | 1:AA:1180:A:H5'    | 1.47                     | 1.14              |
| 35:BA:1821:A:C2'    | 35:BA:1822:G:H5'   | 1.76                     | 1.14              |
| 52:BT:80:SER:HB3    | 52:BT:81:PRO:HD2   | 1.21                     | 1.14              |
| 48:BP:85:LEU:HD21   | 48:BP:117:GLU:O    | 1.34                     | 1.14              |
| 33:B8:62:LEU:HD13   | 35:BA:242:G:H5''   | 1.22                     | 1.14              |
| 35:BA:742:G:C2'     | 35:BA:743:G:H5'    | 1.77                     | 1.14              |
| 35:BA:689:A:C2'     | 35:BA:690:G:H5'    | 1.78                     | 1.14              |
| 9:AI:65:VAL:HG21    | 9:AI:73:GLN:HB3    | 1.24                     | 1.14              |
| 35:BA:1540:U:H3'    | 35:BA:1541:G:H3'   | 1.29                     | 1.14              |
| 1:AA:266:G:C5'      | 1:AA:267:C:C5      | 2.30                     | 1.14              |
| 31:B6:41:PRO:HD2    | 31:B6:46:HIS:H     | 1.02                     | 1.14              |
| 35:BA:2312:U:H2'    | 35:BA:2313:C:H5''  | 1.15                     | 1.14              |
| 1:AA:1175:G:O2'     | 1:AA:1176:A:H5'    | 1.46                     | 1.14              |
| 48:BP:51:PHE:CE2    | 48:BP:53:GLY:CA    | 2.31                     | 1.14              |
| 35:BA:15:G:C2'      | 35:BA:16:G:H5'     | 1.77                     | 1.13              |
| 35:BA:2010:G:C2'    | 35:BA:2011:U:H5'   | 1.78                     | 1.13              |
| 35:BA:1038:C:H3'    | 35:BA:1039:G:H5''  | 1.30                     | 1.13              |
| 1:AA:1281:U:H5'     | 1:AA:1282:C:H5     | 1.08                     | 1.13              |
| 35:BA:1023:U:C2'    | 35:BA:1024:G:H5'   | 1.79                     | 1.13              |
| 35:BA:176:G:C2'     | 35:BA:177:G:H5'    | 1.76                     | 1.13              |
| 35:BA:1988:C:O2'    | 35:BA:1989:G:H5'   | 1.49                     | 1.13              |
| 1:AA:1490:C:C2'     | 1:AA:1491:G:H5'    | 1.79                     | 1.13              |
| 29:B4:32:TYR:O      | 29:B4:33:VAL:HG12  | 1.49                     | 1.13              |
| 35:BA:1890:A:H2'    | 35:BA:1891:G:H5'   | 1.25                     | 1.13              |
| 37:BC:117:THR:H     | 37:BC:118:PRO:CA   | 1.61                     | 1.13              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:BP:23:PRO:HB2  | 48:BP:33:ARG:HE   | 1.11                     | 1.13              |
| 1:AA:1238:A:OP1   | 1:AA:1335:C:H1'   | 1.44                     | 1.12              |
| 35:BA:1381:G:C2'  | 35:BA:1382:G:H5'  | 1.77                     | 1.12              |
| 42:BH:30:LYS:HE2  | 42:BH:81:GLU:HG3  | 1.23                     | 1.12              |
| 52:BT:30:VAL:CB   | 52:BT:31:SER:HB3  | 1.77                     | 1.12              |
| 35:BA:689:A:O2'   | 35:BA:690:G:H5'   | 1.47                     | 1.12              |
| 48:BP:47:ASP:HB3  | 48:BP:48:PRO:C    | 1.68                     | 1.12              |
| 2:AB:87:ARG:NE    | 2:AB:233:SER:OG   | 1.82                     | 1.12              |
| 1:AA:938:A:C2'    | 1:AA:939:G:H5'    | 1.78                     | 1.12              |
| 28:B3:9:VAL:HG11  | 28:B3:55:ARG:HD3  | 1.30                     | 1.12              |
| 31:B6:9:LEU:HD13  | 31:B6:9:LEU:O     | 1.48                     | 1.12              |
| 35:BA:954:G:H2'   | 35:BA:955:C:H5'   | 1.18                     | 1.12              |
| 2:AB:152:PHE:CE1  | 2:AB:155:LEU:HD12 | 1.83                     | 1.12              |
| 27:B2:8:LYS:O     | 27:B2:11:GLU:HG2  | 1.48                     | 1.12              |
| 30:B5:46:CYS:SG   | 30:B5:47:PRO:CD   | 2.37                     | 1.12              |
| 35:BA:743:G:H2'   | 35:BA:744:G:C8    | 1.83                     | 1.12              |
| 52:BT:30:VAL:CG1  | 52:BT:31:SER:HB3  | 1.78                     | 1.12              |
| 9:AI:18:PHE:O     | 9:AI:61:ALA:CA    | 1.97                     | 1.12              |
| 9:AI:19:LEU:HB3   | 9:AI:61:ALA:CB    | 1.80                     | 1.12              |
| 35:BA:2403:C:OP1  | 35:BA:2403:C:H3'  | 1.47                     | 1.12              |
| 19:AS:40:ILE:HD11 | 19:AS:62:ILE:HG13 | 1.32                     | 1.11              |
| 2:AB:122:PHE:HE2  | 2:AB:142:LEU:HD22 | 1.11                     | 1.11              |
| 52:BT:77:PRO:O    | 52:BT:78:LEU:HB2  | 1.49                     | 1.11              |
| 1:AA:1488:G:O2'   | 1:AA:1489:G:H5'   | 1.47                     | 1.11              |
| 1:AA:266:G:H5''   | 1:AA:267:C:H5     | 1.10                     | 1.11              |
| 27:B2:70:GLN:HG2  | 27:B2:71:ASN:H    | 1.03                     | 1.11              |
| 35:BA:1300:U:H4'  | 35:BA:1301:A:O5'  | 1.47                     | 1.11              |
| 35:BA:2363:C:O2'  | 35:BA:2364:C:H5'  | 1.47                     | 1.11              |
| 1:AA:1490:C:H2'   | 1:AA:1491:G:H5'   | 1.15                     | 1.11              |
| 1:AA:349:A:O2'    | 1:AA:350:G:H5'    | 1.46                     | 1.11              |
| 24:AY:69:VAL:HB   | 24:AY:82:ILE:HD11 | 1.23                     | 1.11              |
| 2:AB:228:GLY:HA3  | 2:AB:229:VAL:CG2  | 1.81                     | 1.11              |
| 35:BA:1590:U:H2'  | 35:BA:1591:G:H5'' | 1.30                     | 1.11              |
| 1:AA:1526:G:O2'   | 1:AA:1527:C:H5'   | 1.49                     | 1.11              |
| 9:AI:19:LEU:HA    | 9:AI:61:ALA:CA    | 1.79                     | 1.11              |
| 35:BA:1596:A:H2'  | 35:BA:1597:A:H5'  | 1.26                     | 1.10              |
| 35:BA:37:C:O2'    | 35:BA:38:A:H5'    | 1.50                     | 1.10              |
| 51:BS:97:ARG:HH21 | 51:BS:98:VAL:HA   | 1.14                     | 1.10              |
| 1:AA:1047:G:H2'   | 1:AA:1048:G:H5'   | 1.34                     | 1.10              |
| 2:AB:230:VAL:HB   | 2:AB:231:GLU:HA   | 1.16                     | 1.10              |
| 35:BA:1770:G:O2'  | 35:BA:1771:C:H5'  | 1.51                     | 1.10              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:AI:19:LEU:N      | 9:AI:61:ALA:CB    | 2.15                     | 1.10              |
| 35:BA:523:C:C2'    | 35:BA:524:U:H5'   | 1.80                     | 1.10              |
| 1:AA:543:C:H2'     | 1:AA:544:G:H5'    | 1.15                     | 1.10              |
| 1:AA:88:A:H4'      | 1:AA:89:C:H5'     | 1.20                     | 1.10              |
| 35:BA:963:U:O2'    | 35:BA:964:C:H5'   | 1.51                     | 1.10              |
| 22:AV:40:C:O2'     | 22:AV:41:C:H5'    | 1.52                     | 1.10              |
| 35:BA:612:C:C2'    | 35:BA:613:G:H5''  | 1.82                     | 1.10              |
| 37:BC:117:THR:N    | 37:BC:118:PRO:HA  | 1.57                     | 1.10              |
| 52:BT:80:SER:HB3   | 52:BT:81:PRO:HD3  | 1.24                     | 1.10              |
| 1:AA:264:U:C2'     | 1:AA:265:G:H5'    | 1.80                     | 1.10              |
| 1:AA:938:A:H2'     | 1:AA:939:G:H5'    | 1.30                     | 1.10              |
| 27:B2:70:GLN:CG    | 27:B2:71:ASN:H    | 1.65                     | 1.10              |
| 35:BA:1892:C:C2'   | 35:BA:1893:C:H5'  | 1.81                     | 1.09              |
| 35:BA:2189:U:H2'   | 35:BA:2190:G:H5'' | 1.28                     | 1.09              |
| 1:AA:112:G:C2'     | 1:AA:113:G:H5'    | 1.80                     | 1.09              |
| 1:AA:311:C:H2'     | 1:AA:312:C:C5'    | 1.82                     | 1.09              |
| 35:BA:1970:A:C5'   | 35:BA:1972:A:H1'  | 1.81                     | 1.09              |
| 35:BA:1642:G:H2'   | 35:BA:1643:G:H5'  | 1.33                     | 1.09              |
| 35:BA:2009:G:C2'   | 35:BA:2010:G:H5'  | 1.82                     | 1.09              |
| 37:BC:117:THR:HG21 | 37:BC:119:ASP:HB2 | 1.20                     | 1.09              |
| 41:BG:77:ILE:HG13  | 41:BG:82:LEU:HB2  | 1.31                     | 1.09              |
| 1:AA:1399:C:H4'    | 1:AA:1400:C:O5'   | 1.45                     | 1.09              |
| 41:BG:38:VAL:HG22  | 41:BG:93:THR:HG23 | 1.19                     | 1.09              |
| 1:AA:949:A:H2'     | 1:AA:950:U:H5'    | 1.28                     | 1.09              |
| 27:B2:10:LEU:O     | 27:B2:14:ARG:HD2  | 1.50                     | 1.09              |
| 27:B2:16:LEU:HD22  | 27:B2:20:GLU:HG2  | 1.11                     | 1.09              |
| 35:BA:747:U:C4     | 35:BA:2613:U:C4   | 2.40                     | 1.09              |
| 1:AA:1053:G:H4'    | 1:AA:1054:C:H5'   | 1.16                     | 1.09              |
| 1:AA:1282:C:C2'    | 1:AA:1283:G:H5'   | 1.81                     | 1.09              |
| 35:BA:461:C:H2'    | 35:BA:462:C:H5'   | 1.26                     | 1.09              |
| 1:AA:697:U:H2'     | 1:AA:698:G:H5'    | 1.34                     | 1.09              |
| 1:AA:949:A:C2'     | 1:AA:950:U:H5''   | 1.80                     | 1.09              |
| 24:AY:55:MET:HG2   | 24:AY:56:GLU:N    | 1.64                     | 1.09              |
| 35:BA:1642:G:C2'   | 35:BA:1643:G:H5'  | 1.81                     | 1.09              |
| 35:BA:15:G:O2'     | 35:BA:16:G:H5'    | 1.49                     | 1.09              |
| 35:BA:1983:C:H2'   | 35:BA:1984:G:H5'  | 1.32                     | 1.08              |
| 35:BA:1999:C:C2'   | 35:BA:2000:G:H5'  | 1.81                     | 1.08              |
| 57:BY:28:LYS:HB2   | 57:BY:37:VAL:HB   | 1.32                     | 1.08              |
| 1:AA:696:A:O2'     | 1:AA:697:U:H5'    | 1.54                     | 1.08              |
| 35:BA:2206:G:H21   | 35:BA:2207:G:H5'  | 0.97                     | 1.08              |
| 1:AA:1277:C:O2'    | 1:AA:1279:A:H8    | 1.36                     | 1.08              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1484:G:H2'   | 35:BA:1485:G:H5''  | 1.30                     | 1.08              |
| 58:BZ:180:VAL:HG12 | 58:BZ:181:GLU:H    | 1.14                     | 1.08              |
| 31:B6:27:LYS:HG3   | 31:B6:30:THR:HB    | 1.35                     | 1.08              |
| 35:BA:1988:C:H2'   | 35:BA:1989:G:H5'   | 1.28                     | 1.08              |
| 35:BA:2000:G:N2    | 35:BA:2001:A:C4    | 2.21                     | 1.08              |
| 35:BA:603:A:H1'    | 35:BA:604:G:OP2    | 1.52                     | 1.08              |
| 35:BA:890:A:H3'    | 35:BA:892:G:H5''   | 1.34                     | 1.08              |
| 1:AA:197:A:C6      | 1:AA:221:C:H4'     | 1.88                     | 1.08              |
| 35:BA:1297:C:O2'   | 35:BA:1298:C:H5'   | 1.51                     | 1.08              |
| 35:BA:31:C:C2'     | 35:BA:32:C:H5''    | 1.84                     | 1.08              |
| 24:AY:55:MET:CG    | 24:AY:56:GLU:H     | 1.67                     | 1.07              |
| 35:BA:1806:C:O2'   | 35:BA:1807:G:H5'   | 1.52                     | 1.07              |
| 35:BA:2757:A:H2'   | 35:BA:2758:A:H5'   | 1.32                     | 1.07              |
| 35:BA:612:C:H2'    | 35:BA:613:G:H5''   | 1.14                     | 1.07              |
| 39:BE:132:HIS:HA   | 39:BE:135:HIS:CE1  | 1.89                     | 1.07              |
| 42:BH:3:ARG:CB     | 42:BH:3:ARG:HH11   | 1.66                     | 1.07              |
| 29:B4:21:VAL:HG12  | 29:B4:22:ILE:H     | 1.00                     | 1.07              |
| 35:BA:1215:G:O2'   | 35:BA:1216:G:H5'   | 1.52                     | 1.07              |
| 35:BA:1799:G:H3'   | 35:BA:1799:G:OP1   | 1.53                     | 1.07              |
| 1:AA:1237:C:O2'    | 1:AA:1335:C:O4'    | 1.69                     | 1.07              |
| 42:BH:3:ARG:HB2    | 42:BH:3:ARG:NH1    | 1.70                     | 1.07              |
| 1:AA:1371:G:H2'    | 1:AA:1372:U:H5'    | 1.15                     | 1.07              |
| 27:B2:44:LEU:HD13  | 27:B2:45:SER:N     | 1.70                     | 1.07              |
| 27:B2:44:LEU:HD13  | 27:B2:44:LEU:C     | 1.70                     | 1.07              |
| 35:BA:2757:A:H2'   | 35:BA:2758:A:C5'   | 1.83                     | 1.07              |
| 35:BA:31:C:H2'     | 35:BA:32:C:H5''    | 1.31                     | 1.07              |
| 58:BZ:185:GLU:HG2  | 58:BZ:185:GLU:O    | 1.54                     | 1.07              |
| 1:AA:1498:U:H1'    | 1:AA:1499:A:OP2    | 1.53                     | 1.07              |
| 3:AC:83:ARG:HG3    | 3:AC:84:ILE:N      | 1.69                     | 1.07              |
| 35:BA:1119:C:C2'   | 35:BA:1120:G:H5'   | 1.85                     | 1.07              |
| 35:BA:953:A:H2'    | 35:BA:954:G:H5'    | 1.28                     | 1.07              |
| 1:AA:112:G:H2'     | 1:AA:113:G:H5'     | 1.35                     | 1.07              |
| 35:BA:654(H):G:H2' | 35:BA:654(I):C:H5' | 1.37                     | 1.07              |
| 1:AA:1052:U:O4     | 1:AA:1200:C:H2'    | 1.55                     | 1.07              |
| 27:B2:70:GLN:HG2   | 27:B2:71:ASN:N     | 1.69                     | 1.07              |
| 1:AA:1157:A:H1'    | 1:AA:1158:C:OP2    | 1.52                     | 1.06              |
| 1:AA:560:U:H4'     | 1:AA:561:U:C5'     | 1.85                     | 1.06              |
| 1:AA:264:U:H2'     | 1:AA:265:G:H5'     | 1.31                     | 1.06              |
| 1:AA:311:C:C2'     | 1:AA:312:C:C5'     | 2.33                     | 1.06              |
| 1:AA:1313:U:H3'    | 19:AS:6:LYS:HZ2    | 1.13                     | 1.06              |
| 35:BA:627:A:H4'    | 35:BA:628:G:OP1    | 1.41                     | 1.06              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:172:ILE:HD12  | 2:AB:172:ILE:H    | 1.16                     | 1.06              |
| 2:AB:23:ARG:CG     | 2:AB:23:ARG:HH11  | 1.65                     | 1.06              |
| 35:BA:1600:C:O2'   | 35:BA:1601:G:H5'  | 1.55                     | 1.06              |
| 52:BT:80:SER:CB    | 52:BT:81:PRO:CD   | 2.30                     | 1.06              |
| 58:BZ:180:VAL:HG12 | 58:BZ:181:GLU:N   | 1.68                     | 1.06              |
| 35:BA:1427:A:H4'   | 35:BA:1428:C:O5'  | 1.55                     | 1.06              |
| 29:B4:12:ALA:H     | 29:B4:24:THR:HG22 | 0.96                     | 1.06              |
| 35:BA:2126:A:H4'   | 35:BA:2127:G:O5'  | 1.54                     | 1.06              |
| 36:BB:20:C:H2'     | 36:BB:21:G:H5''   | 1.33                     | 1.06              |
| 35:BA:2105:C:H2'   | 35:BA:2106:G:H5'' | 1.38                     | 1.06              |
| 35:BA:743:G:H2'    | 35:BA:744:G:H8    | 0.92                     | 1.06              |
| 1:AA:521:G:C2'     | 1:AA:522:C:H5'    | 1.84                     | 1.06              |
| 35:BA:1174:A:H5''  | 35:BA:1175:U:H5'' | 1.31                     | 1.06              |
| 35:BA:2645:G:H3'   | 35:BA:2646:C:H5'  | 1.37                     | 1.06              |
| 35:BA:604:G:C2'    | 35:BA:605:C:H5'   | 1.86                     | 1.06              |
| 46:BN:4:TYR:HB3    | 53:BU:64:ARG:HH12 | 1.19                     | 1.06              |
| 3:AC:72:LYS:HG2    | 3:AC:75:VAL:HG23  | 1.07                     | 1.06              |
| 54:BV:62:LEU:HD21  | 54:BV:95:LEU:HB2  | 1.35                     | 1.06              |
| 29:B4:40:HIS:N     | 29:B4:41:PRO:HD2  | 1.71                     | 1.06              |
| 35:BA:1890:A:C2'   | 35:BA:1891:G:H5'  | 1.85                     | 1.06              |
| 1:AA:688:G:O6      | 1:AA:700:G:C6     | 2.09                     | 1.05              |
| 27:B2:9:GLN:H      | 27:B2:9:GLN:CD    | 1.50                     | 1.05              |
| 35:BA:1375:C:O2'   | 35:BA:1376:C:H5'  | 1.53                     | 1.05              |
| 35:BA:742:G:H2'    | 35:BA:743:G:H5'   | 1.07                     | 1.05              |
| 33:B8:13:ARG:HD2   | 48:BP:61:ARG:HD2  | 1.37                     | 1.05              |
| 35:BA:1119:C:O2'   | 35:BA:1120:G:H5'  | 1.56                     | 1.05              |
| 1:AA:949:A:C2'     | 1:AA:950:U:C5'    | 2.34                     | 1.05              |
| 5:AE:31:LEU:HD21   | 5:AE:43:LEU:HD11  | 1.37                     | 1.05              |
| 35:BA:2176:A:H4'   | 35:BA:2177:C:OP1  | 1.53                     | 1.05              |
| 49:BQ:60:ARG:HG3   | 58:BZ:179:ASP:CG  | 1.75                     | 1.05              |
| 1:AA:1281:U:H5'    | 1:AA:1282:C:C5    | 1.91                     | 1.05              |
| 1:AA:266:G:H4'     | 1:AA:267:C:O5'    | 1.48                     | 1.05              |
| 1:AA:266:G:H5''    | 1:AA:267:C:C5     | 1.89                     | 1.05              |
| 29:B4:2:LYS:HE2    | 29:B4:5:ILE:HB    | 1.29                     | 1.05              |
| 1:AA:1073:U:C2'    | 1:AA:1074:G:H5'   | 1.85                     | 1.05              |
| 35:BA:1822:G:H2'   | 35:BA:1823:G:H8   | 1.22                     | 1.05              |
| 35:BA:18:C:C2      | 35:BA:19:C:C5     | 2.43                     | 1.05              |
| 35:BA:955:C:H2'    | 35:BA:956:G:H5'   | 1.06                     | 1.05              |
| 52:BT:29:ARG:O     | 52:BT:30:VAL:HG23 | 1.56                     | 1.05              |
| 25:B0:36:ILE:HG13  | 25:B0:36:ILE:O    | 1.57                     | 1.05              |
| 58:BZ:166:SER:HB2  | 58:BZ:168:GLU:N   | 1.70                     | 1.05              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:15:VAL:HG12  | 2:AB:15:VAL:O      | 1.57                     | 1.05              |
| 52:BT:54:ARG:HA   | 52:BT:59:THR:HB    | 1.34                     | 1.05              |
| 35:BA:1805:U:O2'  | 35:BA:1806:C:H5'   | 1.57                     | 1.05              |
| 35:BA:953:A:O2'   | 35:BA:954:G:H5'    | 1.56                     | 1.05              |
| 1:AA:1505:G:H5''  | 1:AA:1506:U:OP1    | 1.57                     | 1.04              |
| 2:AB:228:GLY:HA3  | 2:AB:229:VAL:HG22  | 1.07                     | 1.04              |
| 24:AY:55:MET:HG2  | 24:AY:56:GLU:H     | 1.10                     | 1.04              |
| 35:BA:1773:A:H2'  | 35:BA:1774:C:H5'   | 1.06                     | 1.04              |
| 35:BA:1797:C:O2   | 35:BA:1822:G:N2    | 1.90                     | 1.04              |
| 35:BA:747:U:N3    | 35:BA:2613:U:C4    | 2.25                     | 1.04              |
| 1:AA:521:G:H2'    | 1:AA:522:C:H5'     | 1.35                     | 1.04              |
| 35:BA:1596:A:O2'  | 35:BA:1597:A:H5'   | 1.54                     | 1.04              |
| 1:AA:495:A:C4'    | 1:AA:496:A:H5'     | 1.88                     | 1.04              |
| 35:BA:18:C:H2'    | 35:BA:19:C:H6      | 1.19                     | 1.04              |
| 1:AA:1047:G:C2'   | 1:AA:1048:G:H5'    | 1.87                     | 1.04              |
| 42:BH:168:PRO:HA  | 42:BH:170:ARG:HH22 | 1.19                     | 1.04              |
| 1:AA:545:C:H2'    | 1:AA:546:G:H5'     | 1.07                     | 1.04              |
| 35:BA:31:C:H2'    | 35:BA:32:C:C5'     | 1.86                     | 1.04              |
| 1:AA:495:A:H4'    | 1:AA:496:A:C5'     | 1.87                     | 1.04              |
| 15:AO:82:ILE:HD11 | 15:AO:88:ARG:HB2   | 1.39                     | 1.04              |
| 31:B6:10:LEU:H    | 31:B6:10:LEU:HD22  | 1.19                     | 1.04              |
| 52:BT:16:ARG:NH2  | 52:BT:82:LEU:O     | 1.91                     | 1.04              |
| 2:AB:231:GLU:HB2  | 2:AB:232:PRO:HD2   | 1.31                     | 1.04              |
| 35:BA:179:G:O2'   | 35:BA:180:G:H5'    | 1.56                     | 1.04              |
| 35:BA:2189:U:C2'  | 35:BA:2190:G:H5''  | 1.88                     | 1.04              |
| 35:BA:955:C:H2'   | 35:BA:956:G:C5'    | 1.87                     | 1.04              |
| 1:AA:560:U:H4'    | 1:AA:561:U:O5'     | 1.53                     | 1.03              |
| 31:B6:19:ARG:HG3  | 31:B6:20:ASN:H     | 0.89                     | 1.03              |
| 35:BA:954:G:O2'   | 35:BA:955:C:H5'    | 1.56                     | 1.03              |
| 52:BT:23:ARG:HB2  | 52:BT:24:PRO:CD    | 1.80                     | 1.03              |
| 35:BA:176:G:H2'   | 35:BA:177:G:H5'    | 1.34                     | 1.03              |
| 1:AA:975:A:H4'    | 1:AA:976:G:H5''    | 1.35                     | 1.03              |
| 5:AE:80:ILE:HD12  | 5:AE:138:ALA:HB1   | 1.41                     | 1.03              |
| 35:BA:1023:U:H2'  | 35:BA:1024:G:H5'   | 1.04                     | 1.03              |
| 58:BZ:166:SER:HB2 | 58:BZ:168:GLU:H    | 0.88                     | 1.03              |
| 15:AO:68:ARG:HB2  | 15:AO:68:ARG:HH11  | 1.20                     | 1.03              |
| 24:AY:69:VAL:HA   | 24:AY:82:ILE:HG12  | 1.38                     | 1.03              |
| 35:BA:1997:G:H2'  | 35:BA:1998:G:H5'   | 1.34                     | 1.03              |
| 35:BA:462:C:C2'   | 35:BA:463:G:H5'    | 1.88                     | 1.03              |
| 35:BA:692:C:O2'   | 35:BA:693:C:H5'    | 1.58                     | 1.03              |
| 52:BT:85:LYS:NZ   | 52:BT:85:LYS:HB3   | 1.70                     | 1.03              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:AA:495:A:O2'      | 1:AA:496:A:H2'    | 1.57                     | 1.03              |
| 1:AA:704:A:H2'      | 1:AA:705:U:H5'    | 1.41                     | 1.03              |
| 9:AI:19:LEU:N       | 9:AI:61:ALA:HB2   | 1.71                     | 1.03              |
| 31:B6:19:ARG:CG     | 31:B6:20:ASN:H    | 1.70                     | 1.03              |
| 1:AA:862:C:H2'      | 1:AA:863:U:H5'    | 1.06                     | 1.03              |
| 35:BA:741:G:O2'     | 35:BA:742:G:H5'   | 1.57                     | 1.03              |
| 1:AA:699:C:C2'      | 1:AA:700:G:H5'    | 1.88                     | 1.03              |
| 40:BF:9:ILE:HG12    | 40:BF:14:PRO:HA   | 1.37                     | 1.03              |
| 28:B3:6:VAL:HG12    | 28:B3:56:VAL:HG22 | 1.41                     | 1.03              |
| 35:BA:256:A:H2'     | 35:BA:257:A:H5'   | 1.40                     | 1.03              |
| 48:BP:65:ARG:HB3    | 48:BP:68:GLN:HE22 | 1.24                     | 1.03              |
| 1:AA:312:C:H2'      | 1:AA:313:A:H8     | 1.17                     | 1.03              |
| 1:AA:522:C:H41      | 12:AL:53:ARG:NH2  | 1.55                     | 1.03              |
| 2:AB:190:THR:O      | 2:AB:191:ASP:HB3  | 1.59                     | 1.03              |
| 29:B4:15:ILE:HD13   | 29:B4:33:VAL:HB   | 1.39                     | 1.03              |
| 35:BA:2581:G:C4     | 35:BA:2610:C:N4   | 2.27                     | 1.03              |
| 1:AA:1282:C:H2'     | 1:AA:1283:G:H5'   | 1.36                     | 1.02              |
| 1:AA:979:C:H2'      | 1:AA:980:C:H5''   | 1.41                     | 1.02              |
| 35:BA:1767:C:C2'    | 35:BA:1768:U:H5'  | 1.88                     | 1.02              |
| 58:BZ:180:VAL:CG1   | 58:BZ:181:GLU:H   | 1.71                     | 1.02              |
| 58:BZ:185:GLU:O     | 58:BZ:187:ALA:N   | 1.91                     | 1.02              |
| 29:B4:40:HIS:H      | 29:B4:41:PRO:HD2  | 1.23                     | 1.02              |
| 35:BA:673:C:H4'     | 40:BF:82:ILE:HD11 | 1.35                     | 1.02              |
| 35:BA:1970:A:H5'    | 35:BA:1972:A:H1'  | 1.08                     | 1.02              |
| 48:BP:59:LEU:HA     | 48:BP:61:ARG:HE   | 1.22                     | 1.02              |
| 35:BA:1747(A):G:C2' | 35:BA:1748:G:H5'' | 1.88                     | 1.02              |
| 35:BA:18:C:H2'      | 35:BA:19:C:C6     | 1.92                     | 1.02              |
| 24:AY:82:ILE:O      | 24:AY:82:ILE:HG22 | 1.59                     | 1.02              |
| 35:BA:1106:G:O2'    | 35:BA:1107:G:H5'  | 1.57                     | 1.02              |
| 35:BA:1892:C:H2'    | 35:BA:1893:C:H5'  | 1.41                     | 1.02              |
| 41:BG:133:LEU:HD11  | 41:BG:157:ILE:HB  | 1.41                     | 1.02              |
| 1:AA:699:C:H2'      | 1:AA:700:G:H5'    | 1.35                     | 1.02              |
| 13:AM:10:PRO:CB     | 13:AM:18:ALA:HB1  | 1.90                     | 1.02              |
| 35:BA:605:C:C2'     | 35:BA:606:U:H5'   | 1.90                     | 1.02              |
| 35:BA:1445:A:C8     | 35:BA:1460:A:C2   | 2.48                     | 1.02              |
| 35:BA:1982:C:C4     | 35:BA:1983:C:N4   | 2.27                     | 1.02              |
| 35:BA:2715:C:H2'    | 35:BA:2716:U:H6   | 1.23                     | 1.02              |
| 52:BT:23:ARG:HB2    | 52:BT:24:PRO:HD2  | 1.38                     | 1.02              |
| 52:BT:30:VAL:HG12   | 52:BT:31:SER:CB   | 1.90                     | 1.02              |
| 55:BW:1:MET:HG2     | 55:BW:2:GLU:H     | 1.25                     | 1.02              |
| 2:AB:87:ARG:NH2     | 2:AB:233:SER:OG   | 1.93                     | 1.02              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1381:G:H2'   | 35:BA:1382:G:H5'   | 1.04                     | 1.02              |
| 35:BA:256:A:C2'    | 35:BA:257:A:H5'    | 1.90                     | 1.02              |
| 34:B9:17:ILE:HG13  | 34:B9:26:ILE:HD12  | 1.41                     | 1.02              |
| 35:BA:1103:A:H5'   | 35:BA:1104:C:OP2   | 1.60                     | 1.02              |
| 35:BA:111:A:H2'    | 35:BA:112:U:C5'    | 1.90                     | 1.01              |
| 35:BA:1983:C:C2'   | 35:BA:1984:G:H5'   | 1.89                     | 1.01              |
| 35:BA:2008:C:H2'   | 35:BA:2009:G:H8    | 1.24                     | 1.01              |
| 48:BP:88:LEU:HD11  | 48:BP:95:VAL:HG21  | 1.40                     | 1.01              |
| 12:AL:27:LEU:HD13  | 12:AL:28:LYS:H     | 1.23                     | 1.01              |
| 35:BA:141:A:H8     | 35:BA:1408:C:HO2'  | 1.07                     | 1.01              |
| 35:BA:2360:A:O2'   | 35:BA:2361:A:H5''  | 1.59                     | 1.01              |
| 3:AC:81:GLY:C      | 3:AC:82:GLU:HG3    | 1.77                     | 1.01              |
| 1:AA:365:U:H3'     | 1:AA:365:U:O2      | 1.60                     | 1.01              |
| 35:BA:2402:C:H4'   | 35:BA:2403:C:O5'   | 1.57                     | 1.01              |
| 48:BP:58:THR:O     | 48:BP:61:ARG:HG2   | 1.58                     | 1.01              |
| 35:BA:1273:U:H5''  | 35:BA:1646:C:N4    | 1.73                     | 1.01              |
| 2:AB:187:LEU:HD22  | 2:AB:187:LEU:O     | 1.59                     | 1.01              |
| 42:BH:106:THR:HG22 | 42:BH:112:PRO:HB3  | 1.42                     | 1.01              |
| 2:AB:87:ARG:HD2    | 2:AB:219:VAL:HG11  | 1.41                     | 1.01              |
| 13:AM:19:LEU:HB3   | 13:AM:25:ILE:HG21  | 1.41                     | 1.01              |
| 35:BA:1799:G:H4'   | 35:BA:1800:C:O5'   | 1.60                     | 1.01              |
| 35:BA:742:G:O2'    | 35:BA:743:G:H5''   | 1.61                     | 1.01              |
| 38:BD:248:SER:HB2  | 38:BD:249:PRO:HD2  | 1.39                     | 1.01              |
| 48:BP:51:PHE:CZ    | 48:BP:53:GLY:HA2   | 1.95                     | 1.01              |
| 1:AA:1030(B):C:H2' | 1:AA:1030(C):G:H4' | 1.39                     | 1.01              |
| 35:BA:2716:U:O2'   | 35:BA:2717:G:H5'   | 1.59                     | 1.01              |
| 1:AA:1388:C:H2'    | 1:AA:1389:C:C6     | 1.95                     | 1.01              |
| 2:AB:23:ARG:HG3    | 2:AB:23:ARG:HH11   | 0.90                     | 1.01              |
| 35:BA:2009:G:H2'   | 35:BA:2010:G:C5'   | 1.91                     | 1.01              |
| 35:BA:326:G:O2'    | 35:BA:327:G:H5'    | 1.59                     | 1.01              |
| 36:BB:40:U:H3'     | 36:BB:41:U:H5''    | 1.41                     | 1.01              |
| 41:BG:137:GLU:HG2  | 41:BG:154:GLY:N    | 1.75                     | 1.01              |
| 2:AB:23:ARG:HG3    | 2:AB:23:ARG:NH1    | 1.66                     | 1.00              |
| 20:AT:74:LYS:HG3   | 20:AT:75:ASN:H     | 1.22                     | 1.00              |
| 35:BA:1446:C:N4    | 35:BA:1465:G:H1    | 1.59                     | 1.00              |
| 35:BA:2128:C:O2'   | 35:BA:2129:C:H5'   | 1.58                     | 1.00              |
| 37:BC:117:THR:HG21 | 37:BC:119:ASP:CB   | 1.91                     | 1.00              |
| 51:BS:106:ARG:HB3  | 51:BS:106:ARG:HH11 | 1.19                     | 1.00              |
| 35:BA:1222:C:C2'   | 35:BA:1223:G:H5'   | 1.91                     | 1.00              |
| 35:BA:860:U:O2'    | 35:BA:861:A:H5'    | 1.61                     | 1.00              |
| 48:BP:51:PHE:HA    | 48:BP:52:GLU:CB    | 1.89                     | 1.00              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:312:C:H2'     | 1:AA:313:A:C8      | 1.95                     | 1.00              |
| 35:BA:16:G:O2'     | 35:BA:17:G:H5'     | 1.60                     | 1.00              |
| 35:BA:2606:C:H2'   | 35:BA:2607:G:H5'   | 1.02                     | 1.00              |
| 25:B0:10:THR:HG22  | 25:B0:11:ARG:H     | 1.24                     | 1.00              |
| 31:B6:19:ARG:HG3   | 31:B6:20:ASN:N     | 1.73                     | 1.00              |
| 38:BD:44:ASN:HB2   | 38:BD:48:ARG:O     | 1.60                     | 1.00              |
| 1:AA:547:A:H1'     | 1:AA:548:G:OP2     | 1.59                     | 1.00              |
| 35:BA:2206:G:N2    | 35:BA:2207:G:H5'   | 1.75                     | 1.00              |
| 35:BA:462:C:O2'    | 35:BA:463:G:H5'    | 1.61                     | 1.00              |
| 50:BR:42:LYS:O     | 50:BR:45:ARG:HG2   | 1.60                     | 1.00              |
| 29:B4:39:CYS:HB3   | 29:B4:41:PRO:HD2   | 1.38                     | 1.00              |
| 35:BA:2009:G:H2'   | 35:BA:2010:G:H5'   | 1.03                     | 1.00              |
| 1:AA:1285:A:H4'    | 1:AA:1286:A:C5'    | 1.91                     | 1.00              |
| 4:AD:139:ARG:HG2   | 4:AD:139:ARG:HH11  | 0.84                     | 1.00              |
| 42:BH:3:ARG:HB2    | 42:BH:3:ARG:HH11   | 1.19                     | 1.00              |
| 50:BR:2:ARG:O      | 50:BR:2:ARG:HD2    | 1.59                     | 1.00              |
| 1:AA:1492:A:H1'    | 1:AA:1493:A:OP1    | 1.62                     | 1.00              |
| 26:B1:29:GLY:O     | 26:B1:30:VAL:HG23  | 1.59                     | 1.00              |
| 39:BE:24:THR:HG21  | 39:BE:188:VAL:HG11 | 1.44                     | 1.00              |
| 4:AD:110:PHE:HD1   | 4:AD:110:PHE:H     | 1.04                     | 1.00              |
| 35:BA:856:C:H2'    | 35:BA:857:C:H6     | 1.02                     | 0.99              |
| 41:BG:137:GLU:HG2  | 41:BG:154:GLY:H    | 1.27                     | 0.99              |
| 1:AA:1154:G:O2'    | 1:AA:1155:G:H5'    | 1.62                     | 0.99              |
| 57:BY:28:LYS:H     | 57:BY:28:LYS:CD    | 1.72                     | 0.99              |
| 2:AB:20:GLU:HG3    | 2:AB:190:THR:O     | 1.63                     | 0.99              |
| 35:BA:1821:A:H2'   | 35:BA:1822:G:H5'   | 1.37                     | 0.99              |
| 35:BA:702:G:C2'    | 35:BA:703:U:H5'    | 1.92                     | 0.99              |
| 1:AA:769:G:C2'     | 1:AA:770:C:H5'     | 1.91                     | 0.99              |
| 39:BE:57:LYS:HA    | 39:BE:57:LYS:HE3   | 1.44                     | 0.99              |
| 52:BT:27:THR:HG23  | 52:BT:28:VAL:H     | 1.24                     | 0.99              |
| 53:BU:90:VAL:HG11  | 54:BV:39:LEU:HG    | 1.45                     | 0.99              |
| 51:BS:35:ILE:H     | 51:BS:53:SER:HB2   | 1.25                     | 0.99              |
| 3:AC:72:LYS:CG     | 3:AC:75:VAL:HG23   | 1.91                     | 0.99              |
| 29:B4:12:ALA:CA    | 29:B4:24:THR:CG2   | 2.29                     | 0.99              |
| 35:BA:2606:C:H2'   | 35:BA:2607:G:C5'   | 1.93                     | 0.99              |
| 35:BA:29:U:O2'     | 35:BA:30:G:H5'     | 1.63                     | 0.99              |
| 15:AO:87:ILE:HG22  | 15:AO:88:ARG:H     | 1.28                     | 0.99              |
| 35:BA:111:A:C2'    | 35:BA:112:U:C5'    | 2.41                     | 0.99              |
| 58:BZ:128:VAL:HG22 | 58:BZ:129:SER:H    | 1.26                     | 0.99              |
| 4:AD:139:ARG:HG2   | 4:AD:139:ARG:NH1   | 1.63                     | 0.98              |
| 35:BA:967:C:H2'    | 35:BA:968:G:H5'    | 0.99                     | 0.98              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 58:BZ:166:SER:CB   | 58:BZ:168:GLU:H   | 1.74                     | 0.98              |
| 1:AA:188:C:H2'     | 1:AA:189:G:C8     | 1.96                     | 0.98              |
| 1:AA:37:U:O2'      | 1:AA:38:G:H5'     | 1.63                     | 0.98              |
| 13:AM:15:VAL:O     | 13:AM:19:LEU:HD23 | 1.63                     | 0.98              |
| 1:AA:197:A:H4'     | 1:AA:198:G:O5'    | 1.57                     | 0.98              |
| 35:BA:1820:U:H4'   | 35:BA:1821:A:OP2  | 1.57                     | 0.98              |
| 1:AA:188:C:H2'     | 1:AA:189:G:H8     | 1.23                     | 0.98              |
| 1:AA:57:G:H2'      | 1:AA:58:C:C6      | 1.98                     | 0.98              |
| 35:BA:967:C:C2'    | 35:BA:968:G:C5'   | 2.41                     | 0.98              |
| 1:AA:119:A:N6      | 1:AA:287:U:O2     | 1.97                     | 0.98              |
| 1:AA:509:A:H5'     | 4:AD:54:TYR:HD2   | 1.23                     | 0.98              |
| 35:BA:1817:G:H2'   | 35:BA:1818:U:H5'  | 1.42                     | 0.98              |
| 37:BC:117:THR:HG22 | 37:BC:118:PRO:O   | 1.61                     | 0.98              |
| 1:AA:593:G:C2'     | 1:AA:594:G:H5'    | 1.94                     | 0.98              |
| 10:AJ:90:LEU:H     | 10:AJ:91:PRO:CD   | 1.76                     | 0.98              |
| 24:AY:264:LEU:HB2  | 61:AY:701:GCP:C5  | 1.93                     | 0.98              |
| 26:B1:5:CYS:SG     | 26:B1:8:SER:N     | 2.37                     | 0.98              |
| 35:BA:655:A:H4'    | 35:BA:656:G:H5'   | 1.42                     | 0.98              |
| 1:AA:951:G:N2      | 1:AA:970:C:O2     | 1.96                     | 0.98              |
| 1:AA:792:A:H4'     | 1:AA:793:U:O5'    | 1.62                     | 0.98              |
| 2:AB:122:PHE:CE2   | 2:AB:142:LEU:HD22 | 1.97                     | 0.98              |
| 27:B2:5:GLU:HA     | 27:B2:8:LYS:HD2   | 1.46                     | 0.98              |
| 35:BA:1590:U:C2'   | 35:BA:1591:G:H5'' | 1.92                     | 0.98              |
| 1:AA:266:G:H5'     | 1:AA:267:C:C5     | 1.99                     | 0.98              |
| 35:BA:145:G:C2'    | 35:BA:146:G:H5''  | 1.94                     | 0.98              |
| 2:AB:15:VAL:HG21   | 2:AB:209:ARG:HH21 | 1.26                     | 0.97              |
| 35:BA:1767:C:H2'   | 35:BA:1768:U:H5'  | 1.43                     | 0.97              |
| 52:BT:30:VAL:HB    | 52:BT:31:SER:HB3  | 1.41                     | 0.97              |
| 1:AA:1002:G:H2'    | 1:AA:1003:G:H8    | 1.26                     | 0.97              |
| 2:AB:17:PHE:HB3    | 2:AB:44:LEU:HD11  | 1.47                     | 0.97              |
| 35:BA:1902:C:O2'   | 38:BD:244:ARG:CB  | 2.10                     | 0.97              |
| 35:BA:653:A:C5'    | 35:BA:654:A:OP2   | 2.11                     | 0.97              |
| 35:BA:743:G:C2'    | 35:BA:744:G:H8    | 1.77                     | 0.97              |
| 1:AA:1371:G:H2'    | 1:AA:1372:U:C5'   | 1.93                     | 0.97              |
| 7:AG:36:LYS:HG2    | 7:AG:37:ASN:H     | 1.28                     | 0.97              |
| 30:B5:4:HIS:HB3    | 30:B5:5:PRO:CD    | 1.89                     | 0.97              |
| 35:BA:1417:C:C2'   | 35:BA:1418:G:H5'  | 1.93                     | 0.97              |
| 35:BA:145:G:H2'    | 35:BA:146:G:H5''  | 1.43                     | 0.97              |
| 35:BA:747:U:C4     | 35:BA:2613:U:N3   | 2.32                     | 0.97              |
| 35:BA:43:A:C2'     | 35:BA:44:G:H5'    | 1.93                     | 0.97              |
| 35:BA:692:C:C2'    | 35:BA:693:C:H5'   | 1.95                     | 0.97              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:742:G:C2'     | 35:BA:743:G:C5'    | 2.40                     | 0.97              |
| 2:AB:228:GLY:CA     | 2:AB:229:VAL:CG2   | 2.38                     | 0.97              |
| 12:AL:46:LYS:C      | 12:AL:48:PRO:HD2   | 1.84                     | 0.97              |
| 24:AY:191:ASP:HB3   | 24:AY:265:LYS:HG3  | 1.46                     | 0.97              |
| 35:BA:742:G:H2'     | 35:BA:743:G:C5'    | 1.93                     | 0.97              |
| 1:AA:796:C:O2'      | 1:AA:797:C:H5'     | 1.65                     | 0.97              |
| 4:AD:139:ARG:CG     | 4:AD:139:ARG:HH11  | 1.77                     | 0.97              |
| 49:BQ:60:ARG:CG     | 58:BZ:179:ASP:OD1  | 2.12                     | 0.97              |
| 1:AA:1285:A:H4'     | 1:AA:1286:A:O5'    | 1.63                     | 0.97              |
| 2:AB:167:PRO:HD3    | 2:AB:188:ALA:HB2   | 1.46                     | 0.97              |
| 12:AL:6:THR:H       | 12:AL:9:GLN:HE21   | 1.08                     | 0.97              |
| 24:AY:31:ARG:NH1    | 24:AY:31:ARG:HA    | 1.79                     | 0.97              |
| 35:BA:2893:G:H5'    | 35:BA:2894:G:H5'   | 1.45                     | 0.97              |
| 35:BA:676:A:H8      | 35:BA:2069:G:H21   | 1.00                     | 0.97              |
| 35:BA:890:A:C3'     | 35:BA:892:G:H5''   | 1.94                     | 0.97              |
| 1:AA:1388:C:H2'     | 1:AA:1389:C:H6     | 1.27                     | 0.97              |
| 1:AA:868:C:O2'      | 1:AA:869:G:H5'     | 1.64                     | 0.97              |
| 35:BA:1770:G:C2'    | 35:BA:1771:C:H5'   | 1.95                     | 0.97              |
| 35:BA:2620:C:H5''   | 39:BE:153:GLY:HA2  | 1.45                     | 0.97              |
| 27:B2:69:ARG:O      | 27:B2:70:GLN:HB3   | 1.65                     | 0.97              |
| 35:BA:2068:U:H3     | 35:BA:2430:A:H2    | 1.01                     | 0.97              |
| 52:BT:30:VAL:HG12   | 52:BT:31:SER:HB3   | 1.42                     | 0.97              |
| 1:AA:508:C:H4'      | 1:AA:509:A:O5'     | 1.62                     | 0.96              |
| 35:BA:1291:C:O2'    | 35:BA:1292:U:H5'   | 1.64                     | 0.96              |
| 1:AA:688:G:C6       | 1:AA:700:G:N1      | 2.32                     | 0.96              |
| 1:AA:701:C:H5'      | 1:AA:702:A:OP1     | 1.63                     | 0.96              |
| 24:AY:201:ILE:H     | 24:AY:201:ILE:HD12 | 1.29                     | 0.96              |
| 1:AA:555:C:C4       | 1:AA:556:C:N4      | 2.33                     | 0.96              |
| 2:AB:200:ILE:HD12   | 2:AB:200:ILE:H     | 1.30                     | 0.96              |
| 26:B1:57:GLU:HG2    | 26:B1:58:ILE:N     | 1.77                     | 0.96              |
| 1:AA:1073:U:H2'     | 1:AA:1074:G:H5'    | 1.45                     | 0.96              |
| 24:AY:137:ASN:ND2   | 24:AY:138:LYS:H    | 1.63                     | 0.96              |
| 39:BE:77:ILE:HG22   | 39:BE:78:LEU:H     | 1.29                     | 0.96              |
| 1:AA:1053:G:H4'     | 1:AA:1054:C:C5'    | 1.96                     | 0.96              |
| 35:BA:271(L):U:H5'' | 35:BA:271(M):G:H5' | 1.46                     | 0.96              |
| 35:BA:741:G:C2'     | 35:BA:742:G:H5'    | 1.95                     | 0.96              |
| 1:AA:1150:U:H2'     | 1:AA:1151:A:H5'    | 1.47                     | 0.96              |
| 20:AT:73:HIS:O      | 20:AT:74:LYS:HG2   | 1.64                     | 0.96              |
| 35:BA:1282:U:O2     | 35:BA:1286:A:N6    | 1.99                     | 0.96              |
| 35:BA:2207:G:H5''   | 35:BA:2207:G:N3    | 1.80                     | 0.96              |
| 37:BC:117:THR:CG2   | 37:BC:118:PRO:C    | 2.32                     | 0.96              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:B4:22:ILE:HG12 | 41:BG:105:LYS:HA   | 1.47                     | 0.96              |
| 40:BF:178:PRO:HB2 | 40:BF:201:VAL:HG11 | 1.46                     | 0.96              |
| 35:BA:84:A:H5''   | 57:BY:9:LYS:HD2    | 1.47                     | 0.96              |
| 1:AA:1029:C:H3'   | 1:AA:1030:C:H5''   | 1.47                     | 0.96              |
| 1:AA:1282:C:O2'   | 1:AA:1283:G:H5'    | 1.64                     | 0.96              |
| 35:BA:2358:G:C2'  | 35:BA:2359:C:H5'   | 1.95                     | 0.96              |
| 35:BA:2713:A:H3'  | 35:BA:2714:G:H5'   | 1.47                     | 0.96              |
| 35:BA:650:C:H3'   | 35:BA:651:G:H5''   | 1.45                     | 0.96              |
| 35:BA:896:A:H1'   | 58:BZ:176:PRO:CG   | 1.95                     | 0.96              |
| 35:BA:2010:G:H2'  | 35:BA:2011:U:H5'   | 1.43                     | 0.96              |
| 38:BD:24:ILE:HG23 | 38:BD:25:THR:H     | 1.30                     | 0.96              |
| 57:BY:101:LYS:HG2 | 57:BY:102:CYS:N    | 1.79                     | 0.96              |
| 9:AI:19:LEU:HB3   | 9:AI:61:ALA:HB3    | 1.46                     | 0.96              |
| 35:BA:1997:G:C2'  | 35:BA:1998:G:H5'   | 1.96                     | 0.96              |
| 58:BZ:149:SER:CB  | 58:BZ:173:ALA:HA   | 1.96                     | 0.96              |
| 1:AA:106:C:HO2'   | 1:AA:107:G:H5'     | 1.21                     | 0.95              |
| 1:AA:1303:C:H2'   | 1:AA:1304:G:H5'    | 1.47                     | 0.95              |
| 19:AS:29:ARG:HB3  | 19:AS:48:THR:HB    | 1.48                     | 0.95              |
| 35:BA:1067:A:H5'' | 35:BA:1068:G:H5''  | 1.45                     | 0.95              |
| 35:BA:330:A:H2    | 35:BA:1210:A:H2'   | 1.30                     | 0.95              |
| 35:BA:53:A:H2'    | 35:BA:54:G:H5'     | 1.43                     | 0.95              |
| 27:B2:64:LEU:HD23 | 27:B2:64:LEU:O     | 1.64                     | 0.95              |
| 35:BA:27:G:N2     | 35:BA:512:G:H2'    | 1.81                     | 0.95              |
| 39:BE:179:GLU:HB3 | 39:BE:181:LEU:HD23 | 1.44                     | 0.95              |
| 58:BZ:5:LEU:HD23  | 58:BZ:47:VAL:HG21  | 1.44                     | 0.95              |
| 1:AA:60:A:H4'     | 1:AA:61:G:O5'      | 1.64                     | 0.95              |
| 40:BF:24:LEU:HB3  | 40:BF:25:PRO:HD2   | 1.48                     | 0.95              |
| 1:AA:312:C:O2'    | 1:AA:313:A:H5'     | 1.67                     | 0.95              |
| 1:AA:949:A:O2'    | 1:AA:950:U:H5''    | 1.65                     | 0.95              |
| 35:BA:689:A:H2'   | 35:BA:690:G:H5'    | 1.48                     | 0.95              |
| 1:AA:348:G:H2'    | 1:AA:349:A:H5'     | 1.47                     | 0.95              |
| 35:BA:630:G:N2    | 35:BA:633:A:OP2    | 1.99                     | 0.95              |
| 35:BA:967:C:H2'   | 35:BA:968:G:C5'    | 1.96                     | 0.95              |
| 39:BE:36:ARG:HH21 | 39:BE:88:GLY:HA2   | 1.31                     | 0.95              |
| 13:AM:7:VAL:HG21  | 41:BG:147:ASP:OD1  | 1.67                     | 0.95              |
| 35:BA:111:A:H2'   | 35:BA:112:U:H5'    | 0.97                     | 0.95              |
| 26:B1:45:ASN:HD21 | 35:BA:2090:G:H21   | 1.14                     | 0.95              |
| 35:BA:2355:C:H2'  | 35:BA:2356:C:H5'   | 1.46                     | 0.95              |
| 48:BP:47:ASP:OD2  | 48:BP:49:ARG:HB2   | 1.65                     | 0.95              |
| 1:AA:1153:C:O2'   | 1:AA:1154:G:H5''   | 1.66                     | 0.95              |
| 1:AA:491:G:H2'    | 1:AA:492:G:H8      | 1.32                     | 0.95              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 4:AD:17:VAL:HG12    | 4:AD:18:LYS:H     | 1.29                     | 0.95              |
| 35:BA:2126:A:H1'    | 35:BA:2127:G:O4'  | 1.67                     | 0.95              |
| 1:AA:1399:C:OP2     | 1:AA:1399:C:H2'   | 1.65                     | 0.95              |
| 12:AL:27:LEU:HD12   | 12:AL:28:LYS:HE2  | 1.44                     | 0.95              |
| 35:BA:1899:G:H21    | 35:BA:1902:C:H41  | 1.00                     | 0.95              |
| 35:BA:2606:C:C2'    | 35:BA:2607:G:C5'  | 2.44                     | 0.95              |
| 35:BA:604:G:O2'     | 35:BA:605:C:H5'   | 1.66                     | 0.95              |
| 35:BA:954:G:H2'     | 35:BA:955:C:C5'   | 1.97                     | 0.94              |
| 35:BA:461:C:C2'     | 35:BA:462:C:H5'   | 1.96                     | 0.94              |
| 35:BA:53:A:C2'      | 35:BA:54:G:H5'    | 1.97                     | 0.94              |
| 35:BA:2756:U:H1'    | 35:BA:2757:A:OP2  | 1.67                     | 0.94              |
| 35:BA:612:C:H2'     | 35:BA:613:G:C5'   | 1.96                     | 0.94              |
| 3:AC:138:VAL:HG21   | 3:AC:168:ALA:CB   | 1.98                     | 0.94              |
| 8:AH:89:PRO:HA      | 8:AH:92:ARG:HH11  | 1.32                     | 0.94              |
| 13:AM:101:GLN:HE21  | 13:AM:101:GLN:H   | 1.12                     | 0.94              |
| 48:BP:47:ASP:CB     | 48:BP:48:PRO:HA   | 1.96                     | 0.94              |
| 51:BS:13:ARG:HG3    | 51:BS:14:VAL:H    | 1.32                     | 0.94              |
| 52:BT:79:HIS:O      | 52:BT:80:SER:HB2  | 1.64                     | 0.94              |
| 51:BS:54:LEU:HD13   | 51:BS:57:LYS:HA   | 1.48                     | 0.94              |
| 2:AB:187:LEU:C      | 2:AB:187:LEU:HD22 | 1.87                     | 0.94              |
| 10:AJ:34:VAL:HG22   | 10:AJ:74:ILE:HG22 | 1.49                     | 0.94              |
| 1:AA:173:U:H5'      | 1:AA:197:A:O4'    | 1.65                     | 0.94              |
| 35:BA:1528(A):A:H62 | 35:BA:1541:G:N2   | 1.65                     | 0.94              |
| 48:BP:23:PRO:CB     | 48:BP:33:ARG:HE   | 1.81                     | 0.94              |
| 30:B5:3:LYS:HD3     | 35:BA:2611:U:O2'  | 1.68                     | 0.94              |
| 35:BA:1058:G:H2'    | 35:BA:1059:G:H5'' | 1.48                     | 0.94              |
| 35:BA:2306:C:O2     | 41:BG:45:GLU:HA   | 1.68                     | 0.94              |
| 35:BA:329:G:H1      | 57:BY:19:LYS:HE3  | 1.33                     | 0.94              |
| 6:AF:24:GLU:HG2     | 6:AF:28:ARG:HH12  | 1.30                     | 0.94              |
| 24:AY:454:MET:H     | 24:AY:458:HIS:HD2 | 1.06                     | 0.94              |
| 28:B3:9:VAL:CG1     | 28:B3:55:ARG:CD   | 2.44                     | 0.94              |
| 40:BF:84:VAL:HG22   | 40:BF:85:GLY:H    | 1.31                     | 0.94              |
| 1:AA:1368:G:H2'     | 1:AA:1369:C:H5'   | 1.49                     | 0.94              |
| 30:B5:40:LYS:CE     | 30:B5:46:CYS:HB3  | 1.98                     | 0.94              |
| 1:AA:198:G:C6       | 1:AA:220:G:C2     | 2.55                     | 0.93              |
| 1:AA:522:C:C2'      | 1:AA:523:A:H5'    | 1.97                     | 0.93              |
| 1:AA:769:G:H2'      | 1:AA:770:C:H5'    | 1.47                     | 0.93              |
| 3:AC:53:ALA:HB2     | 3:AC:115:LEU:HD13 | 1.50                     | 0.93              |
| 29:B4:40:HIS:N      | 29:B4:41:PRO:CD   | 2.30                     | 0.93              |
| 33:B8:59:LYS:HB2    | 33:B8:59:LYS:HZ3  | 1.32                     | 0.93              |
| 48:BP:23:PRO:HB2    | 48:BP:33:ARG:NE   | 1.82                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:AI:19:LEU:CB    | 9:AI:61:ALA:CB    | 2.23                     | 0.93              |
| 35:BA:697:C:HO2'  | 35:BA:698:C:H5'   | 1.25                     | 0.93              |
| 2:AB:228:GLY:HA2  | 2:AB:229:VAL:HG13 | 0.94                     | 0.93              |
| 17:AQ:9:VAL:HG12  | 17:AQ:56:VAL:HG22 | 1.47                     | 0.93              |
| 25:B0:51:VAL:HG21 | 25:B0:79:VAL:O    | 1.68                     | 0.93              |
| 29:B4:39:CYS:O    | 29:B4:40:HIS:HB2  | 1.68                     | 0.93              |
| 35:BA:178:G:C2'   | 35:BA:179:G:H5'   | 1.97                     | 0.93              |
| 35:BA:327:G:O2'   | 35:BA:328:U:H5'   | 1.68                     | 0.93              |
| 48:BP:51:PHE:CE2  | 48:BP:53:GLY:HA3  | 2.03                     | 0.93              |
| 54:BV:24:LYS:HA   | 54:BV:92:THR:HG23 | 1.51                     | 0.93              |
| 12:AL:33:ARG:HD3  | 12:AL:62:SER:HB3  | 1.49                     | 0.93              |
| 28:B3:19:GLN:NE2  | 28:B3:52:HIS:HE1  | 1.66                     | 0.93              |
| 35:BA:600:G:O2'   | 35:BA:601:C:H5'   | 1.67                     | 0.93              |
| 39:BE:54:GLN:O    | 39:BE:55:ASN:HB2  | 1.68                     | 0.93              |
| 1:AA:198:G:O6     | 1:AA:220:G:N1     | 2.01                     | 0.93              |
| 48:BP:47:ASP:HB3  | 48:BP:48:PRO:HA   | 1.48                     | 0.93              |
| 57:BY:28:LYS:HA   | 57:BY:38:ILE:HG22 | 1.51                     | 0.93              |
| 35:BA:1773:A:H2'  | 35:BA:1774:C:C5'  | 1.97                     | 0.93              |
| 35:BA:2716:U:C2'  | 35:BA:2717:G:H5'  | 1.97                     | 0.93              |
| 35:BA:693:C:H2'   | 35:BA:694:U:C6    | 2.03                     | 0.93              |
| 52:BT:85:LYS:HB3  | 52:BT:85:LYS:HZ2  | 1.26                     | 0.93              |
| 1:AA:1371:G:O2'   | 1:AA:1372:U:H5'   | 1.67                     | 0.93              |
| 1:AA:49:U:C2      | 1:AA:361:G:N2     | 2.37                     | 0.93              |
| 31:B6:9:LEU:HD13  | 31:B6:9:LEU:C     | 1.88                     | 0.93              |
| 37:BC:117:THR:CG2 | 37:BC:119:ASP:CB  | 2.45                     | 0.93              |
| 51:BS:106:ARG:HD2 | 51:BS:108:GLY:H   | 1.31                     | 0.93              |
| 1:AA:961:U:H1'    | 1:AA:962:C:H5'    | 1.49                     | 0.93              |
| 31:B6:41:PRO:HD2  | 31:B6:46:HIS:N    | 1.82                     | 0.93              |
| 1:AA:788:U:O2'    | 1:AA:789:U:H5'    | 1.68                     | 0.93              |
| 31:B6:7:ILE:HG21  | 31:B6:27:LYS:HZ3  | 1.07                     | 0.93              |
| 42:BH:171:LEU:O   | 42:BH:173:PRO:HD3 | 1.69                     | 0.93              |
| 1:AA:1238:A:P     | 1:AA:1335:C:H1'   | 2.09                     | 0.92              |
| 2:AB:223:ILE:HG22 | 2:AB:227:GLY:O    | 1.69                     | 0.92              |
| 24:AY:115:GLU:O   | 24:AY:118:SER:HB3 | 1.69                     | 0.92              |
| 35:BA:2032:G:H21  | 39:BE:146:THR:CG2 | 1.80                     | 0.92              |
| 1:AA:73:G:H1      | 1:AA:96:U:H3      | 0.99                     | 0.92              |
| 1:AA:1029:C:H3'   | 1:AA:1030:C:C5'   | 2.00                     | 0.92              |
| 2:AB:152:PHE:CZ   | 2:AB:155:LEU:HD12 | 2.05                     | 0.92              |
| 24:AY:99:ARG:HH11 | 24:AY:402:ILE:N   | 1.68                     | 0.92              |
| 35:BA:1416:G:O2'  | 35:BA:1417:C:H5   | 1.50                     | 0.92              |
| 35:BA:27:G:N2     | 35:BA:512:G:C2'   | 2.32                     | 0.92              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:673:C:C4'    | 40:BF:82:ILE:HD11 | 1.98                     | 0.92              |
| 35:BA:1190:G:H5'   | 48:BP:35:HIS:H    | 1.31                     | 0.92              |
| 51:BS:15:ARG:HH11  | 51:BS:15:ARG:HB2  | 1.32                     | 0.92              |
| 2:AB:230:VAL:CB    | 2:AB:231:GLU:HA   | 1.94                     | 0.92              |
| 18:AR:32:ARG:HA    | 18:AR:69:THR:HG21 | 1.49                     | 0.92              |
| 19:AS:63:THR:HG23  | 19:AS:64:GLU:H    | 1.32                     | 0.92              |
| 35:BA:1381:G:H2'   | 35:BA:1382:G:C5'  | 1.97                     | 0.92              |
| 38:BD:44:ASN:HB3   | 38:BD:49:ILE:HA   | 1.51                     | 0.92              |
| 53:BU:91:ASP:OD1   | 53:BU:96:ALA:HB2  | 1.70                     | 0.92              |
| 3:AC:138:VAL:HG21  | 3:AC:168:ALA:HB1  | 1.51                     | 0.92              |
| 28:B3:9:VAL:HG11   | 28:B3:55:ARG:HD2  | 1.48                     | 0.92              |
| 13:AM:8:GLU:OE1    | 13:AM:22:ILE:HA   | 1.70                     | 0.92              |
| 35:BA:2008:C:H2'   | 35:BA:2009:G:C8   | 2.05                     | 0.92              |
| 1:AA:964:A:N6      | 1:AA:965:A:N6     | 2.17                     | 0.92              |
| 48:BP:47:ASP:CB    | 48:BP:48:PRO:CA   | 2.47                     | 0.92              |
| 50:BR:3:HIS:O      | 50:BR:5:LYS:N     | 2.03                     | 0.92              |
| 52:BT:28:VAL:HG13  | 52:BT:29:ARG:N    | 1.81                     | 0.92              |
| 1:AA:1049:U:H4'    | 1:AA:1050:G:O5'   | 1.66                     | 0.92              |
| 1:AA:60:A:H1'      | 1:AA:61:G:O4'     | 1.70                     | 0.92              |
| 1:AA:688:G:C6      | 1:AA:700:G:C6     | 2.58                     | 0.92              |
| 29:B4:16:CYS:HA    | 29:B4:33:VAL:HG21 | 1.52                     | 0.92              |
| 35:BA:747:U:N3     | 35:BA:2613:U:O4   | 2.01                     | 0.92              |
| 27:B2:44:LEU:CD1   | 27:B2:44:LEU:C    | 2.37                     | 0.92              |
| 35:BA:1649:G:O2'   | 35:BA:1650:G:H5'  | 1.69                     | 0.92              |
| 35:BA:2176:A:H2'   | 35:BA:2177:C:C6   | 2.05                     | 0.92              |
| 1:AA:556:C:H2'     | 1:AA:557:G:H5'    | 1.51                     | 0.92              |
| 24:AY:534:ILE:HD11 | 24:AY:570:GLY:HA3 | 1.49                     | 0.92              |
| 29:B4:21:VAL:HG12  | 29:B4:22:ILE:N    | 1.83                     | 0.92              |
| 35:BA:1899:G:N2    | 35:BA:1902:C:H41  | 1.68                     | 0.92              |
| 37:BC:103:LYS:HE3  | 37:BC:107:GLY:HA3 | 1.50                     | 0.92              |
| 39:BE:60:ASN:OD1   | 39:BE:62:PRO:HD2  | 1.66                     | 0.92              |
| 57:BY:7:VAL:HB     | 57:BY:8:LYS:NZ    | 1.85                     | 0.92              |
| 35:BA:954:G:C2'    | 35:BA:955:C:C5'   | 2.47                     | 0.91              |
| 1:AA:673:G:H2'     | 1:AA:674:G:C8     | 2.05                     | 0.91              |
| 1:AA:964:A:N6      | 1:AA:965:A:H62    | 1.69                     | 0.91              |
| 29:B4:33:VAL:HG13  | 29:B4:34:GLU:N    | 1.80                     | 0.91              |
| 30:B5:47:PRO:HG2   | 30:B5:48:GLU:OE1  | 1.68                     | 0.91              |
| 35:BA:1720:U:C2'   | 35:BA:1721:G:H5'' | 2.00                     | 0.91              |
| 48:BP:146:VAL:HG22 | 48:BP:147:LEU:H   | 1.34                     | 0.91              |
| 1:AA:1371:G:C2'    | 1:AA:1372:U:C5'   | 2.48                     | 0.91              |
| 1:AA:704:A:C2'     | 1:AA:705:U:H5'    | 1.99                     | 0.91              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:112:LYS:HG3  | 9:AI:118:LYS:HA    | 1.50                     | 0.91              |
| 35:BA:1104:C:H2'  | 35:BA:1105:U:H5'   | 1.49                     | 0.91              |
| 35:BA:1540:U:C3'  | 35:BA:1541:G:H3'   | 1.98                     | 0.91              |
| 48:BP:84:ASN:ND2  | 48:BP:116:GLY:CA   | 2.33                     | 0.91              |
| 48:BP:52:GLU:HG2  | 48:BP:57:THR:CG2   | 2.00                     | 0.91              |
| 13:AM:22:ILE:HG21 | 13:AM:66:LEU:HD23  | 1.53                     | 0.91              |
| 17:AQ:67:LYS:HA   | 17:AQ:70:ARG:HH12  | 1.33                     | 0.91              |
| 35:BA:1104:C:C2'  | 35:BA:1105:U:H5'   | 1.99                     | 0.91              |
| 50:BR:99:LYS:HD2  | 50:BR:99:LYS:H     | 1.35                     | 0.91              |
| 2:AB:130:ARG:HH22 | 2:AB:134:GLU:HG3   | 1.36                     | 0.91              |
| 24:AY:497:PHE:O   | 24:AY:507:TYR:HB2  | 1.69                     | 0.91              |
| 29:B4:56:VAL:HA   | 29:B4:60:GLN:CD    | 1.91                     | 0.91              |
| 39:BE:36:ARG:HH21 | 39:BE:88:GLY:CA    | 1.82                     | 0.91              |
| 1:AA:1279:A:H3'   | 1:AA:1279:A:N3     | 1.84                     | 0.91              |
| 7:AG:15:ASP:HB3   | 7:AG:19:GLY:O      | 1.71                     | 0.91              |
| 29:B4:56:VAL:HG22 | 29:B4:57:GLU:H     | 1.32                     | 0.91              |
| 35:BA:2362:G:O2'  | 35:BA:2363:C:H5'   | 1.70                     | 0.91              |
| 24:AY:99:ARG:HD3  | 24:AY:401:SER:HA   | 1.51                     | 0.91              |
| 26:B1:29:GLY:C    | 26:B1:30:VAL:HG23  | 1.89                     | 0.91              |
| 30:B5:53:ALA:HA   | 30:B5:56:LYS:NZ    | 1.84                     | 0.91              |
| 46:BN:24:GLY:O    | 46:BN:28:THR:HG23  | 1.69                     | 0.91              |
| 53:BU:34:LYS:HE2  | 53:BU:34:LYS:HA    | 1.50                     | 0.91              |
| 1:AA:1148:U:C2'   | 1:AA:1149:C:H5'    | 2.00                     | 0.91              |
| 1:AA:1368:G:C2'   | 1:AA:1369:C:H5'    | 1.99                     | 0.91              |
| 1:AA:314:C:O2'    | 1:AA:315:A:H5'     | 1.70                     | 0.91              |
| 12:AL:45:PRO:HG2  | 12:AL:51:ALA:N     | 1.86                     | 0.91              |
| 29:B4:60:GLN:HB2  | 29:B4:62:ARG:NH1   | 1.85                     | 0.91              |
| 35:BA:2029:G:O6   | 35:BA:2033:A:OP1   | 1.88                     | 0.91              |
| 35:BA:953:A:N6    | 35:BA:965:C:N4     | 2.17                     | 0.91              |
| 1:AA:1386:G:C2    | 1:AA:1387:G:N7     | 2.38                     | 0.91              |
| 1:AA:353:A:H5'    | 1:AA:353:A:H8      | 1.34                     | 0.91              |
| 31:B6:7:ILE:CG2   | 31:B6:27:LYS:NZ    | 2.32                     | 0.91              |
| 35:BA:2312:U:C2'  | 35:BA:2313:C:H5''  | 1.98                     | 0.91              |
| 35:BA:2409:G:O2'  | 35:BA:2410:G:H5'   | 1.71                     | 0.91              |
| 22:AV:18:G:O2'    | 22:AV:57:G:N2      | 2.02                     | 0.91              |
| 28:B3:19:GLN:HE22 | 28:B3:52:HIS:HE1   | 1.01                     | 0.91              |
| 38:BD:69:ARG:HD3  | 38:BD:105:ILE:HD11 | 1.53                     | 0.91              |
| 1:AA:186:C:O2'    | 1:AA:187:C:H5'     | 1.71                     | 0.90              |
| 22:AV:41:C:C2'    | 22:AV:42:C:H5'     | 2.00                     | 0.90              |
| 35:BA:1216:G:O2'  | 35:BA:1217:C:H5'   | 1.70                     | 0.90              |
| 35:BA:1994:C:O2'  | 35:BA:1995:U:H5'   | 1.71                     | 0.90              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:697:C:C2'    | 35:BA:698:C:H5'   | 2.00                     | 0.90              |
| 48:BP:16:ARG:HB2   | 48:BP:16:ARG:NH1  | 1.85                     | 0.90              |
| 1:AA:115:G:H1'     | 1:AA:116:A:OP2    | 1.70                     | 0.90              |
| 1:AA:1387:G:O2'    | 1:AA:1388:C:H5'   | 1.70                     | 0.90              |
| 29:B4:15:ILE:O     | 29:B4:16:CYS:HB2  | 1.69                     | 0.90              |
| 35:BA:2713:A:H3'   | 35:BA:2714:G:C5'  | 2.00                     | 0.90              |
| 38:BD:24:ILE:HG23  | 38:BD:25:THR:N    | 1.86                     | 0.90              |
| 58:BZ:97:GLU:HG3   | 58:BZ:127:LYS:HB3 | 1.52                     | 0.90              |
| 35:BA:2124:G:H5''  | 37:BC:175:PRO:HG3 | 1.54                     | 0.90              |
| 52:BT:28:VAL:HG22  | 52:BT:45:PHE:O    | 1.30                     | 0.90              |
| 53:BU:92:ARG:HD3   | 53:BU:94:ASN:HB3  | 1.52                     | 0.90              |
| 1:AA:1279:A:H5''   | 1:AA:1280:A:OP1   | 1.71                     | 0.90              |
| 4:AD:17:VAL:HG12   | 4:AD:18:LYS:N     | 1.85                     | 0.90              |
| 35:BA:176:G:O2'    | 35:BA:177:G:H5'   | 1.69                     | 0.90              |
| 35:BA:1984:G:C2'   | 35:BA:1985:G:H5'  | 2.01                     | 0.90              |
| 35:BA:925:C:H2'    | 35:BA:926:A:H5''  | 1.53                     | 0.90              |
| 35:BA:1484:G:C2'   | 35:BA:1485:G:H5'' | 2.02                     | 0.90              |
| 1:AA:155:C:H2'     | 1:AA:156:G:H8     | 1.35                     | 0.90              |
| 9:AI:19:LEU:N      | 9:AI:61:ALA:HB1   | 1.84                     | 0.90              |
| 25:B0:45:PHE:HE1   | 25:B0:77:ARG:HE   | 1.17                     | 0.90              |
| 26:B1:75:GLU:O     | 26:B1:78:LYS:HG2  | 1.70                     | 0.90              |
| 35:BA:1455:G:C2'   | 35:BA:1456:G:H5'  | 2.01                     | 0.90              |
| 52:BT:16:ARG:HB3   | 52:BT:16:ARG:HH11 | 1.35                     | 0.90              |
| 58:BZ:165:VAL:HG12 | 58:BZ:167:PRO:HA  | 1.54                     | 0.90              |
| 2:AB:167:PRO:HD2   | 2:AB:188:ALA:HB2  | 1.49                     | 0.90              |
| 29:B4:60:GLN:HB2   | 29:B4:62:ARG:HH11 | 1.37                     | 0.90              |
| 41:BG:59:GLU:HG3   | 41:BG:60:LEU:H    | 1.37                     | 0.90              |
| 1:AA:187:C:O2'     | 1:AA:188:C:H5'    | 1.72                     | 0.90              |
| 35:BA:15:G:H2'     | 35:BA:16:G:H5'    | 1.53                     | 0.90              |
| 35:BA:1884:A:H2'   | 35:BA:1885:A:H5'' | 1.50                     | 0.90              |
| 50:BR:2:ARG:HG3    | 50:BR:2:ARG:HH11  | 1.34                     | 0.90              |
| 51:BS:34:HIS:HB3   | 51:BS:53:SER:HB3  | 1.53                     | 0.90              |
| 1:AA:775:G:C2'     | 1:AA:776:G:H5'    | 2.02                     | 0.90              |
| 33:B8:59:LYS:HB2   | 33:B8:59:LYS:NZ   | 1.85                     | 0.90              |
| 35:BA:55:G:N2      | 35:BA:115:C:O2    | 2.04                     | 0.90              |
| 40:BF:84:VAL:CG2   | 40:BF:85:GLY:N    | 2.33                     | 0.90              |
| 57:BY:42:VAL:HG21  | 57:BY:67:LEU:HD13 | 1.52                     | 0.90              |
| 1:AA:1391:U:H2'    | 1:AA:1392:G:C8    | 2.07                     | 0.90              |
| 20:AT:75:ASN:HD22  | 20:AT:75:ASN:H    | 1.15                     | 0.90              |
| 35:BA:1786:A:H1'   | 35:BA:1938:A:N6   | 1.86                     | 0.90              |
| 35:BA:2000:G:C2    | 35:BA:2001:A:C8   | 2.60                     | 0.90              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2656:U:H3    | 35:BA:2665:A:H2    | 1.15                     | 0.90              |
| 38:BD:27:THR:HG23  | 38:BD:83:GLU:HG2   | 1.54                     | 0.90              |
| 52:BT:28:VAL:CG2   | 52:BT:45:PHE:O     | 2.19                     | 0.90              |
| 35:BA:629:G:H2'    | 35:BA:630:G:H5'    | 1.52                     | 0.89              |
| 3:AC:120:VAL:O     | 3:AC:123:GLN:HB2   | 1.72                     | 0.89              |
| 24:AY:454:MET:H    | 24:AY:458:HIS:CD2  | 1.91                     | 0.89              |
| 35:BA:1963:U:H2'   | 35:BA:1963:U:O2    | 1.70                     | 0.89              |
| 35:BA:27:G:H22     | 35:BA:512:G:H2'    | 1.36                     | 0.89              |
| 40:BF:160:ASN:HD21 | 40:BF:162:LEU:HD13 | 1.34                     | 0.89              |
| 48:BP:52:GLU:HG2   | 48:BP:57:THR:HG22  | 1.53                     | 0.89              |
| 1:AA:491:G:H2'     | 1:AA:492:G:C8      | 2.07                     | 0.89              |
| 1:AA:938:A:O2'     | 1:AA:939:G:H5'     | 1.73                     | 0.89              |
| 35:BA:17:G:H2'     | 35:BA:18:C:C6      | 2.06                     | 0.89              |
| 1:AA:1152:A:O2'    | 1:AA:1153:C:H5'    | 1.72                     | 0.89              |
| 9:AI:95:LYS:HE3    | 9:AI:96:LEU:HD22   | 1.54                     | 0.89              |
| 29:B4:21:VAL:CG1   | 29:B4:22:ILE:H     | 1.86                     | 0.89              |
| 35:BA:1076:C:H4'   | 58:BZ:112:ARG:CZ   | 2.02                     | 0.89              |
| 35:BA:2105:C:C2'   | 35:BA:2106:G:H5''  | 2.01                     | 0.89              |
| 37:BC:31:LYS:NZ    | 37:BC:181:PHE:O    | 2.06                     | 0.89              |
| 24:AY:526:VAL:HB   | 24:AY:566:THR:HA   | 1.51                     | 0.89              |
| 1:AA:859:A:C2'     | 1:AA:860:A:H5'     | 2.03                     | 0.89              |
| 35:BA:1799:G:H1'   | 35:BA:1800:C:OP2   | 1.70                     | 0.89              |
| 35:BA:1970:A:H5'   | 35:BA:1972:A:C1'   | 2.01                     | 0.89              |
| 35:BA:2129:C:N4    | 35:BA:2159:G:O6    | 2.04                     | 0.89              |
| 52:BT:78:LEU:O     | 52:BT:79:HIS:HD2   | 1.54                     | 0.89              |
| 1:AA:204:U:H4'     | 1:AA:216:G:O5'     | 1.72                     | 0.89              |
| 30:B5:2:ALA:HA     | 35:BA:2015:A:H1'   | 1.55                     | 0.89              |
| 2:AB:82:ARG:O      | 2:AB:86:GLU:HG3    | 1.71                     | 0.89              |
| 35:BA:178:G:H2'    | 35:BA:179:G:H5'    | 1.54                     | 0.89              |
| 35:BA:2131:G:N2    | 35:BA:2133:A:C2    | 2.40                     | 0.89              |
| 37:BC:121:MET:HA   | 37:BC:124:VAL:HG12 | 1.55                     | 0.89              |
| 52:BT:29:ARG:NH1   | 52:BT:88:ILE:HD11  | 1.87                     | 0.89              |
| 1:AA:364:A:O2'     | 1:AA:365:U:H5'     | 1.73                     | 0.89              |
| 1:AA:522:C:H2'     | 1:AA:523:A:H5'     | 1.53                     | 0.89              |
| 3:AC:72:LYS:HG2    | 3:AC:75:VAL:CG2    | 1.97                     | 0.89              |
| 12:AL:18:VAL:HG23  | 12:AL:19:ARG:H     | 1.38                     | 0.89              |
| 33:B8:28:GLY:O     | 33:B8:32:LEU:HD23  | 1.70                     | 0.89              |
| 37:BC:117:THR:H    | 37:BC:118:PRO:HA   | 0.74                     | 0.89              |
| 35:BA:2032:G:H21   | 39:BE:146:THR:HG23 | 1.36                     | 0.89              |
| 41:BG:77:ILE:HG23  | 41:BG:80:PHE:HB2   | 1.52                     | 0.89              |
| 58:BZ:151:HIS:HB2  | 58:BZ:170:THR:HA   | 1.53                     | 0.89              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:4:ILE:HG22   | 13:AM:5:ALA:N      | 1.88                     | 0.89              |
| 24:AY:546:ILE:HG23 | 24:AY:590:ILE:HG13 | 1.54                     | 0.89              |
| 35:BA:155:U:H2'    | 35:BA:156:U:H5''   | 1.51                     | 0.89              |
| 35:BA:910:A:H62    | 49:BQ:12:GLN:HA    | 1.37                     | 0.89              |
| 38:BD:35:LYS:H     | 38:BD:36:PRO:CD    | 1.85                     | 0.89              |
| 1:AA:40:C:O2'      | 1:AA:41:G:H5'      | 1.73                     | 0.88              |
| 25:B0:7:LEU:HD13   | 49:BQ:85:LYS:HE2   | 1.53                     | 0.88              |
| 48:BP:59:LEU:HA    | 48:BP:61:ARG:NE    | 1.87                     | 0.88              |
| 1:AA:697:U:C2'     | 1:AA:698:G:H5'     | 2.02                     | 0.88              |
| 25:B0:43:THR:O     | 25:B0:43:THR:HG23  | 1.72                     | 0.88              |
| 35:BA:262:A:O2'    | 35:BA:263:C:H5'    | 1.73                     | 0.88              |
| 35:BA:30:G:H2'     | 35:BA:31:C:C6      | 2.08                     | 0.88              |
| 48:BP:50:ARG:O     | 48:BP:52:GLU:HB2   | 1.71                     | 0.88              |
| 52:BT:23:ARG:CB    | 52:BT:24:PRO:CD    | 2.49                     | 0.88              |
| 1:AA:322:C:O2'     | 1:AA:323:U:H5'     | 1.72                     | 0.88              |
| 1:AA:862:C:C2'     | 1:AA:863:U:C5'     | 2.52                     | 0.88              |
| 33:B8:56:GLU:HA    | 33:B8:59:LYS:HZ1   | 1.38                     | 0.88              |
| 48:BP:77:ARG:HD3   | 48:BP:78:PRO:HD2   | 1.53                     | 0.88              |
| 57:BY:8:LYS:N      | 57:BY:8:LYS:HD2    | 1.88                     | 0.88              |
| 1:AA:1238:A:OP1    | 1:AA:1335:C:O2'    | 1.91                     | 0.88              |
| 4:AD:7:PRO:HB2     | 4:AD:10:ARG:HD2    | 1.54                     | 0.88              |
| 35:BA:856:C:C2'    | 35:BA:857:C:H6     | 1.87                     | 0.88              |
| 54:BV:15:GLU:HG3   | 54:BV:16:PRO:HD2   | 1.56                     | 0.88              |
| 1:AA:1285:A:H4'    | 1:AA:1286:A:H5'    | 1.55                     | 0.88              |
| 35:BA:332:A:H1'    | 35:BA:333:G:OP1    | 1.74                     | 0.88              |
| 35:BA:743:G:O2'    | 35:BA:744:G:H5'    | 1.74                     | 0.88              |
| 35:BA:953:A:N6     | 35:BA:965:C:H42    | 1.72                     | 0.88              |
| 35:BA:1902:C:C2'   | 38:BD:244:ARG:HB2  | 2.03                     | 0.88              |
| 38:BD:30:GLU:HG3   | 38:BD:63:ARG:CZ    | 2.04                     | 0.88              |
| 1:AA:593:G:HO2'    | 1:AA:594:G:H5'     | 1.35                     | 0.88              |
| 27:B2:10:LEU:O     | 27:B2:14:ARG:HB2   | 1.73                     | 0.88              |
| 27:B2:70:GLN:HE21  | 27:B2:71:ASN:N     | 1.72                     | 0.88              |
| 1:AA:548:G:C2'     | 1:AA:549:C:H5'     | 2.04                     | 0.88              |
| 31:B6:25:LYS:HE2   | 33:B8:34:TRP:HE1   | 1.39                     | 0.88              |
| 41:BG:139:LEU:HB3  | 41:BG:153:ARG:O    | 1.74                     | 0.88              |
| 47:BO:4:PRO:O      | 47:BO:5:GLN:HB2    | 1.71                     | 0.88              |
| 31:B6:52:VAL:HG22  | 31:B6:53:LYS:H     | 1.39                     | 0.88              |
| 35:BA:2681:C:H5    | 35:BA:2725:A:H62   | 1.19                     | 0.88              |
| 39:BE:141:ILE:CA   | 39:BE:154:LYS:HE2  | 2.03                     | 0.88              |
| 41:BG:77:ILE:HG13  | 41:BG:82:LEU:CB    | 2.02                     | 0.88              |
| 28:B3:9:VAL:CG1    | 28:B3:55:ARG:HD2   | 2.03                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:197:A:N6     | 1:AA:221:C:H4'    | 1.88                     | 0.88              |
| 32:B7:8:ASN:HD22  | 32:B7:8:ASN:C     | 1.78                     | 0.88              |
| 35:BA:179:G:C2'   | 35:BA:180:G:C5'   | 2.51                     | 0.88              |
| 35:BA:179:G:H2'   | 35:BA:180:G:C5'   | 2.04                     | 0.88              |
| 1:AA:1127:G:H1    | 1:AA:1145:C:H42   | 1.20                     | 0.87              |
| 1:AA:1184:G:O2'   | 1:AA:1185:G:H5'   | 1.74                     | 0.87              |
| 1:AA:1229:A:H8    | 1:AA:1229:A:H5'   | 1.36                     | 0.87              |
| 1:AA:1330:U:H3'   | 1:AA:1331:G:O4'   | 1.74                     | 0.87              |
| 28:B3:1:MET:HB3   | 28:B3:2:PRO:HD2   | 1.56                     | 0.87              |
| 35:BA:1120:G:O2'  | 35:BA:1121:C:H5'  | 1.73                     | 0.87              |
| 35:BA:2147:G:H2'  | 35:BA:2148:G:O4'  | 1.74                     | 0.87              |
| 25:B0:14:ARG:HG2  | 25:B0:14:ARG:HH11 | 1.39                     | 0.87              |
| 31:B6:10:LEU:CD2  | 31:B6:10:LEU:N    | 2.30                     | 0.87              |
| 35:BA:1332:G:N2   | 35:BA:1609:A:O2'  | 2.07                     | 0.87              |
| 1:AA:173:U:H5''   | 1:AA:197:A:H5'    | 1.57                     | 0.87              |
| 20:AT:75:ASN:N    | 20:AT:75:ASN:HD22 | 1.66                     | 0.87              |
| 24:AY:618:GLY:HA3 | 35:BA:1095:A:OP1  | 1.75                     | 0.87              |
| 28:B3:9:VAL:CG1   | 28:B3:55:ARG:HD3  | 2.02                     | 0.87              |
| 35:BA:1890:A:H2'  | 35:BA:1891:G:C5'  | 2.03                     | 0.87              |
| 35:BA:2127:G:H2'  | 35:BA:2128:C:H5'  | 1.54                     | 0.87              |
| 1:AA:774:G:HO2'   | 1:AA:775:G:H5'    | 1.36                     | 0.87              |
| 35:BA:2029:G:H1   | 35:BA:2033:A:P    | 1.98                     | 0.87              |
| 35:BA:2180:U:H6   | 35:BA:2180:U:H5'  | 1.39                     | 0.87              |
| 42:BH:3:ARG:HB3   | 42:BH:6:ARG:HB2   | 1.56                     | 0.87              |
| 1:AA:522:C:O2'    | 1:AA:523:A:H5'    | 1.74                     | 0.87              |
| 24:AY:84:THR:HG21 | 24:AY:94:VAL:HG22 | 1.56                     | 0.87              |
| 35:BA:2393:A:H4'  | 48:BP:61:ARG:O    | 1.74                     | 0.87              |
| 51:BS:30:ARG:HD3  | 51:BS:97:ARG:HG2  | 1.54                     | 0.87              |
| 1:AA:1076:C:O2'   | 1:AA:1077:G:H5'   | 1.73                     | 0.87              |
| 1:AA:1307:U:H2'   | 1:AA:1308:U:C6    | 2.09                     | 0.87              |
| 27:B2:41:ILE:HD12 | 27:B2:43:GLN:HG3  | 1.56                     | 0.87              |
| 50:BR:45:ARG:HG3  | 50:BR:46:GLY:H    | 1.37                     | 0.87              |
| 58:BZ:48:PHE:HE2  | 58:BZ:74:VAL:HG21 | 1.37                     | 0.87              |
| 1:AA:1313:U:H3'   | 19:AS:6:LYS:NZ    | 1.90                     | 0.87              |
| 2:AB:16:HIS:HE1   | 2:AB:210:SER:O    | 1.58                     | 0.87              |
| 2:AB:228:GLY:C    | 2:AB:229:VAL:HG22 | 1.91                     | 0.87              |
| 35:BA:2207:G:O2'  | 35:BA:2208:A:H5'' | 1.74                     | 0.87              |
| 35:BA:896:A:H1'   | 58:BZ:176:PRO:HG3 | 1.56                     | 0.87              |
| 37:BC:124:VAL:O   | 37:BC:128:LEU:HB3 | 1.75                     | 0.87              |
| 48:BP:112:LEU:H   | 48:BP:128:HIS:HD2 | 1.19                     | 0.87              |
| 54:BV:1:MET:O     | 54:BV:2:PHE:HB3   | 1.72                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:83:ARG:HG3    | 3:AC:84:ILE:H      | 1.37                     | 0.87              |
| 35:BA:462:C:H2'    | 35:BA:463:G:H5'    | 1.56                     | 0.87              |
| 35:BA:699:A:C2'    | 35:BA:700:G:H5'    | 2.05                     | 0.87              |
| 35:BA:968:G:HO2'   | 35:BA:969:U:H5'    | 1.37                     | 0.87              |
| 38:BD:35:LYS:O     | 38:BD:35:LYS:HD2   | 1.73                     | 0.87              |
| 47:BO:13:ASN:HD21  | 47:BO:96:THR:H     | 1.20                     | 0.87              |
| 58:BZ:151:HIS:HA   | 58:BZ:171:ILE:HG12 | 1.57                     | 0.87              |
| 1:AA:688:G:O6      | 1:AA:700:G:N1      | 2.08                     | 0.87              |
| 31:B6:11:LEU:H     | 31:B6:11:LEU:HD13  | 1.39                     | 0.87              |
| 1:AA:46:G:O2'      | 1:AA:365:U:H1'     | 1.75                     | 0.86              |
| 1:AA:560:U:H4'     | 1:AA:561:U:H5''    | 1.55                     | 0.86              |
| 35:BA:1412:A:O2'   | 35:BA:1413:G:H5'   | 1.73                     | 0.86              |
| 35:BA:1821:A:O2'   | 35:BA:1822:G:H5'   | 1.74                     | 0.86              |
| 35:BA:1892:C:O2'   | 35:BA:1893:C:H5'   | 1.73                     | 0.86              |
| 35:BA:272(I):U:H6  | 35:BA:272(I):U:H5' | 1.40                     | 0.86              |
| 46:BN:12:ARG:HH21  | 46:BN:135:PRO:HG2  | 1.37                     | 0.86              |
| 2:AB:155:LEU:HD21  | 2:AB:159:PRO:HG3   | 1.57                     | 0.86              |
| 6:AF:24:GLU:HG2    | 6:AF:28:ARG:NH1    | 1.89                     | 0.86              |
| 35:BA:2000:G:O2'   | 35:BA:2001:A:H5'   | 1.73                     | 0.86              |
| 35:BA:43:A:O2'     | 35:BA:44:G:H5'     | 1.75                     | 0.86              |
| 1:AA:106:C:C2'     | 1:AA:107:G:H5'     | 2.05                     | 0.86              |
| 26:B1:57:GLU:HG2   | 26:B1:58:ILE:H     | 1.38                     | 0.86              |
| 29:B4:39:CYS:HB3   | 29:B4:41:PRO:CD    | 2.05                     | 0.86              |
| 35:BA:2715:C:H2'   | 35:BA:2716:U:C6    | 2.11                     | 0.86              |
| 35:BA:958:U:OP2    | 49:BQ:14:ARG:NH1   | 2.07                     | 0.86              |
| 57:BY:42:VAL:HG12  | 57:BY:65:ALA:HB3   | 1.57                     | 0.86              |
| 1:AA:112:G:O2'     | 1:AA:113:G:H5'     | 1.75                     | 0.86              |
| 1:AA:1305:G:HO2'   | 1:AA:1306:A:H8     | 0.91                     | 0.86              |
| 1:AA:547:A:H4'     | 1:AA:548:G:O5'     | 1.76                     | 0.86              |
| 7:AG:115:ARG:O     | 7:AG:118:VAL:HG12  | 1.76                     | 0.86              |
| 35:BA:1023:U:H2'   | 35:BA:1024:G:C5'   | 2.00                     | 0.86              |
| 35:BA:2392:A:H2    | 35:BA:2424:C:H42   | 1.18                     | 0.86              |
| 57:BY:28:LYS:HB2   | 57:BY:38:ILE:H     | 1.41                     | 0.86              |
| 1:AA:105:G:H2'     | 1:AA:106:C:C6      | 2.11                     | 0.86              |
| 29:B4:56:VAL:HA    | 29:B4:60:GLN:NE2   | 1.90                     | 0.86              |
| 35:BA:528:A:C2     | 35:BA:2042:A:H2'   | 2.11                     | 0.86              |
| 24:AY:238:THR:HG22 | 24:AY:241:GLU:HG2  | 1.56                     | 0.86              |
| 25:B0:66:VAL:O     | 25:B0:81:VAL:HG13  | 1.76                     | 0.86              |
| 35:BA:1822:G:H2'   | 35:BA:1823:G:C8    | 2.11                     | 0.86              |
| 35:BA:2580:U:H5'   | 39:BE:131:ALA:HB2  | 1.58                     | 0.86              |
| 13:AM:7:VAL:CG2    | 41:BG:147:ASP:OD1  | 2.24                     | 0.86              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BN:128:HIS:CD2 | 46:BN:130:HIS:H    | 1.92                     | 0.86              |
| 50:BR:7:GLY:HA3   | 50:BR:8:ARG:NH2    | 1.90                     | 0.86              |
| 1:AA:558:G:H2'    | 1:AA:559:A:H2      | 1.40                     | 0.86              |
| 1:AA:940:C:C2'    | 1:AA:941:G:H5'     | 2.05                     | 0.86              |
| 28:B3:8:LEU:HD13  | 28:B3:31:LEU:HD23  | 1.56                     | 0.86              |
| 35:BA:2029:G:C6   | 35:BA:2033:A:OP1   | 2.28                     | 0.86              |
| 35:BA:2787:C:H1'  | 39:BE:61:ARG:HH11  | 1.38                     | 0.86              |
| 46:BN:133:GLN:HG2 | 46:BN:134:ARG:H    | 1.41                     | 0.86              |
| 1:AA:1238:A:OP1   | 1:AA:1335:C:C2'    | 2.24                     | 0.86              |
| 1:AA:37:U:C2'     | 1:AA:38:G:C5'      | 2.53                     | 0.86              |
| 1:AA:61:G:O2'     | 1:AA:62:U:H5'      | 1.75                     | 0.86              |
| 35:BA:1890:A:C3'  | 35:BA:1891:G:H5'   | 2.06                     | 0.86              |
| 35:BA:604:G:H2'   | 35:BA:605:C:H5'    | 1.54                     | 0.86              |
| 35:BA:914:C:H2'   | 35:BA:915:C:H5'    | 1.54                     | 0.86              |
| 41:BG:39:ILE:HD12 | 41:BG:157:ILE:HG12 | 1.55                     | 0.86              |
| 50:BR:118:GLU:HA  | 50:BR:118:GLU:OE1  | 1.75                     | 0.86              |
| 52:BT:32:TYR:O    | 52:BT:33:LYS:HB2   | 1.75                     | 0.86              |
| 1:AA:1305:G:OP1   | 21:AU:2:GLY:HA2    | 1.73                     | 0.86              |
| 1:AA:308:C:H2'    | 1:AA:309:G:H8      | 1.39                     | 0.86              |
| 10:AJ:4:ILE:HD13  | 10:AJ:77:PRO:HG3   | 1.57                     | 0.86              |
| 35:BA:32:C:O2'    | 35:BA:33:U:H5'     | 1.76                     | 0.86              |
| 40:BF:11:VAL:HG12 | 40:BF:12:LEU:HG    | 1.56                     | 0.86              |
| 1:AA:1077:G:N1    | 1:AA:1081:G:C6     | 2.44                     | 0.86              |
| 1:AA:1388:C:O2'   | 1:AA:1389:C:H5'    | 1.75                     | 0.86              |
| 37:BC:52:PRO:HG2  | 37:BC:53:ARG:HD3   | 1.57                     | 0.86              |
| 1:AA:311:C:H2'    | 1:AA:312:C:H5'     | 0.86                     | 0.85              |
| 35:BA:1494:A:C2'  | 35:BA:1495:A:H5"   | 2.06                     | 0.85              |
| 12:AL:83:VAL:HG11 | 12:AL:100:ILE:HG12 | 1.58                     | 0.85              |
| 15:AO:68:ARG:CB   | 15:AO:68:ARG:HH11  | 1.89                     | 0.85              |
| 31:B6:10:LEU:HD23 | 31:B6:10:LEU:H     | 1.40                     | 0.85              |
| 35:BA:693:C:O2'   | 35:BA:694:U:H5'    | 1.74                     | 0.85              |
| 42:BH:83:TYR:HB3  | 42:BH:134:SER:HA   | 1.58                     | 0.85              |
| 48:BP:57:THR:C    | 48:BP:59:LEU:H     | 1.79                     | 0.85              |
| 1:AA:1523:G:C2'   | 1:AA:1524:C:H5'    | 2.06                     | 0.85              |
| 1:AA:522:C:N4     | 12:AL:53:ARG:NH2   | 2.24                     | 0.85              |
| 1:AA:773:G:HO2'   | 1:AA:774:G:H5'     | 1.40                     | 0.85              |
| 1:AA:980:C:H5'    | 1:AA:980:C:H6      | 1.40                     | 0.85              |
| 2:AB:204:ASN:ND2  | 2:AB:206:ASP:H     | 1.74                     | 0.85              |
| 2:AB:231:GLU:CB   | 2:AB:232:PRO:CD    | 2.48                     | 0.85              |
| 10:AJ:54:PHE:CE2  | 10:AJ:55:LYS:HD2   | 2.09                     | 0.85              |
| 31:B6:17:LYS:HB2  | 31:B6:18:ARG:HH11  | 1.41                     | 0.85              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:1819:A:OP1  | 38:BD:158:ALA:N    | 2.09                     | 0.85              |
| 35:BA:1988:C:C2'  | 35:BA:1989:G:C5'   | 2.52                     | 0.85              |
| 56:BX:8:ILE:HD11  | 56:BX:42:ALA:HB1   | 1.56                     | 0.85              |
| 1:AA:1498:U:H4'   | 1:AA:1499:A:O5'    | 1.76                     | 0.85              |
| 19:AS:41:VAL:HB   | 19:AS:44:MET:HB3   | 1.56                     | 0.85              |
| 35:BA:27:G:N2     | 35:BA:512:G:O2'    | 2.08                     | 0.85              |
| 35:BA:528:A:N1    | 35:BA:2042:A:H2'   | 1.92                     | 0.85              |
| 54:BV:39:LEU:HD12 | 54:BV:47:VAL:HG11  | 1.58                     | 0.85              |
| 24:AY:109:ASP:OD1 | 24:AY:138:LYS:HD2  | 1.77                     | 0.85              |
| 35:BA:111:A:O2'   | 35:BA:112:U:H5'    | 1.73                     | 0.85              |
| 35:BA:1988:C:H2'  | 35:BA:1989:G:C5'   | 2.07                     | 0.85              |
| 35:BA:653:A:H3'   | 35:BA:653:A:N3     | 1.91                     | 0.85              |
| 48:BP:16:ARG:CZ   | 48:BP:18:ARG:HG2   | 2.06                     | 0.85              |
| 35:BA:2757:A:C2'  | 35:BA:2758:A:C5'   | 2.54                     | 0.85              |
| 36:BB:7:G:H2'     | 36:BB:8:U:H5"      | 1.59                     | 0.85              |
| 40:BF:89:VAL:HG12 | 40:BF:90:PHE:N     | 1.90                     | 0.85              |
| 48:BP:16:ARG:HB2  | 48:BP:16:ARG:HH11  | 1.37                     | 0.85              |
| 35:BA:2009:G:OP1  | 55:BW:41:LYS:HE2   | 1.76                     | 0.85              |
| 1:AA:509:A:H3'    | 1:AA:509:A:OP2     | 1.76                     | 0.85              |
| 10:AJ:33:GLN:HB2  | 10:AJ:75:ILE:HG12  | 1.58                     | 0.85              |
| 32:B7:34:ARG:HH11 | 32:B7:34:ARG:HG3   | 1.41                     | 0.85              |
| 35:BA:1779:U:H5   | 35:BA:1784:A:N7    | 1.74                     | 0.85              |
| 35:BA:526:A:O2'   | 35:BA:2043:C:O2'   | 1.93                     | 0.85              |
| 41:BG:59:GLU:HG3  | 41:BG:60:LEU:N     | 1.90                     | 0.85              |
| 35:BA:629:G:C2'   | 35:BA:630:G:H5'    | 2.06                     | 0.85              |
| 13:AM:91:ARG:HB3  | 13:AM:98:VAL:HG12  | 1.57                     | 0.85              |
| 35:BA:1379:A:H4'  | 35:BA:1380:G:OP2   | 1.77                     | 0.85              |
| 26:B1:29:GLY:CA   | 35:BA:2396:G:O2'   | 2.24                     | 0.85              |
| 48:BP:51:PHE:CD2  | 48:BP:52:GLU:O     | 2.30                     | 0.85              |
| 1:AA:1127:G:H1    | 1:AA:1145:C:N4     | 1.73                     | 0.85              |
| 1:AA:495:A:O4'    | 1:AA:496:A:C8      | 2.30                     | 0.85              |
| 2:AB:17:PHE:CD1   | 2:AB:17:PHE:C      | 2.44                     | 0.85              |
| 35:BA:2032:G:N2   | 39:BE:146:THR:HG23 | 1.92                     | 0.85              |
| 35:BA:2712:U:O2'  | 35:BA:2713:A:H5'   | 1.76                     | 0.85              |
| 2:AB:17:PHE:C     | 2:AB:17:PHE:HD1    | 1.76                     | 0.84              |
| 27:B2:16:LEU:O    | 27:B2:17:SER:HB3   | 1.75                     | 0.84              |
| 35:BA:2127:G:O2'  | 35:BA:2128:C:H5"   | 1.76                     | 0.84              |
| 52:BT:80:SER:CB   | 52:BT:81:PRO:HD3   | 2.01                     | 0.84              |
| 1:AA:1157:A:H4'   | 1:AA:1158:C:O5'    | 1.77                     | 0.84              |
| 9:AI:53:VAL:HG22  | 9:AI:95:LYS:HZ3    | 1.40                     | 0.84              |
| 61:AY:701:GCP:O1G | 62:AY:2002:HOH:O   | 1.94                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BF:25:PRO:HB3   | 40:BF:119:ARG:HB2  | 1.59                     | 0.84              |
| 41:BG:105:LYS:HE2  | 41:BG:105:LYS:N    | 1.92                     | 0.84              |
| 1:AA:1002:G:H2'    | 1:AA:1003:G:C8     | 2.12                     | 0.84              |
| 1:AA:949:A:H2'     | 1:AA:950:U:H5''    | 1.42                     | 0.84              |
| 3:AC:40:ARG:O      | 3:AC:44:GLU:HG2    | 1.77                     | 0.84              |
| 25:B0:29:GLN:O     | 25:B0:67:VAL:HG23  | 1.76                     | 0.84              |
| 41:BG:141:PHE:HD1  | 41:BG:142:PRO:HA   | 1.42                     | 0.84              |
| 57:BY:28:LYS:CB    | 57:BY:37:VAL:HB    | 2.07                     | 0.84              |
| 1:AA:1124:G:H5'    | 10:AJ:35:SER:HB2   | 1.60                     | 0.84              |
| 1:AA:1182:G:OP2    | 1:AA:1182:G:C8     | 2.30                     | 0.84              |
| 1:AA:682:G:H5''    | 38:BD:169:GLU:OE1  | 1.78                     | 0.84              |
| 24:AY:69:VAL:HA    | 24:AY:82:ILE:CG1   | 2.07                     | 0.84              |
| 30:B5:40:LYS:NZ    | 30:B5:46:CYS:HB3   | 1.91                     | 0.84              |
| 40:BF:157:VAL:HG13 | 40:BF:194:MET:HG2  | 1.57                     | 0.84              |
| 56:BX:35:THR:HG22  | 56:BX:37:THR:H     | 1.42                     | 0.84              |
| 57:BY:96:ILE:HG21  | 57:BY:99:CYS:SG    | 2.18                     | 0.84              |
| 1:AA:264:U:H2'     | 1:AA:265:G:C5'     | 2.07                     | 0.84              |
| 9:AI:23:ASN:N      | 9:AI:23:ASN:HD22   | 1.75                     | 0.84              |
| 29:B4:12:ALA:H     | 29:B4:24:THR:CB    | 1.88                     | 0.84              |
| 35:BA:1412:A:C2'   | 35:BA:1413:G:H5'   | 2.07                     | 0.84              |
| 1:AA:348:G:C2'     | 1:AA:349:A:H5'     | 2.08                     | 0.84              |
| 2:AB:204:ASN:HD22  | 2:AB:205:ASP:N     | 1.76                     | 0.84              |
| 3:AC:22:TRP:CE3    | 3:AC:22:TRP:O      | 2.30                     | 0.84              |
| 7:AG:56:GLN:O      | 7:AG:57:GLU:HB3    | 1.78                     | 0.84              |
| 35:BA:1455:G:H2'   | 35:BA:1456:G:H5'   | 1.57                     | 0.84              |
| 35:BA:2009:G:C2'   | 35:BA:2010:G:C5'   | 2.51                     | 0.84              |
| 40:BF:84:VAL:HG22  | 40:BF:85:GLY:N     | 1.91                     | 0.84              |
| 58:BZ:149:SER:HB2  | 58:BZ:173:ALA:HA   | 1.57                     | 0.84              |
| 1:AA:264:U:O2'     | 1:AA:265:G:H5'     | 1.76                     | 0.84              |
| 2:AB:16:HIS:O      | 2:AB:17:PHE:CG     | 2.30                     | 0.84              |
| 24:AY:530:VAL:HG22 | 24:AY:531:GLY:H    | 1.40                     | 0.84              |
| 25:B0:62:LEU:HD23  | 25:B0:62:LEU:N     | 1.93                     | 0.84              |
| 35:BA:1865:G:H8    | 35:BA:1865:G:H5'   | 1.42                     | 0.84              |
| 1:AA:1175:G:C2'    | 1:AA:1176:A:H5'    | 2.06                     | 0.84              |
| 2:AB:82:ARG:HA     | 2:AB:92:TYR:CZ     | 2.13                     | 0.84              |
| 31:B6:27:LYS:CG    | 31:B6:30:THR:HB    | 2.08                     | 0.84              |
| 35:BA:1460:A:O2'   | 35:BA:1461:G:H5'   | 1.77                     | 0.84              |
| 35:BA:699:A:H2'    | 35:BA:700:G:H5'    | 1.60                     | 0.84              |
| 35:BA:1803:A:O2'   | 38:BD:259:THR:HG21 | 1.78                     | 0.84              |
| 1:AA:1488:G:HO2'   | 1:AA:1489:G:H5'    | 1.40                     | 0.84              |
| 1:AA:1523:G:H2'    | 1:AA:1524:C:H5'    | 1.60                     | 0.84              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:173:U:C2      | 1:AA:197:A:C2     | 2.66                     | 0.84              |
| 10:AJ:44:VAL:HG22  | 10:AJ:66:ARG:HG2  | 1.59                     | 0.84              |
| 25:B0:19:LYS:NZ    | 25:B0:41:ARG:HH22 | 1.75                     | 0.84              |
| 35:BA:1119:C:H2'   | 35:BA:1120:G:H5'  | 1.57                     | 0.84              |
| 35:BA:1297:C:O2    | 35:BA:1643:G:N2   | 2.11                     | 0.84              |
| 38:BD:267:SER:O    | 38:BD:269:PHE:N   | 2.11                     | 0.84              |
| 1:AA:773:G:C2'     | 1:AA:774:G:H5'    | 2.08                     | 0.84              |
| 1:AA:191:G:C4      | 20:AT:105:SER:HB3 | 2.13                     | 0.84              |
| 35:BA:2787:C:H1'   | 39:BE:61:ARG:HG3  | 1.60                     | 0.84              |
| 38:BD:32:SER:O     | 38:BD:36:PRO:HD3  | 1.78                     | 0.84              |
| 1:AA:1400:C:H4'    | 1:AA:1401:G:OP2   | 1.74                     | 0.83              |
| 1:AA:495:A:C1'     | 1:AA:496:A:C8     | 2.60                     | 0.83              |
| 7:AG:50:ILE:HD11   | 7:AG:61:VAL:HB    | 1.58                     | 0.83              |
| 24:AY:252:ASP:HB3  | 24:AY:254:LYS:NZ  | 1.93                     | 0.83              |
| 25:B0:11:ARG:HD3   | 25:B0:12:ASN:H    | 1.41                     | 0.83              |
| 35:BA:1106:G:C2'   | 35:BA:1107:G:H5'  | 2.07                     | 0.83              |
| 35:BA:1228:G:N2    | 35:BA:1229:G:H1'  | 1.93                     | 0.83              |
| 35:BA:528:A:O2'    | 35:BA:529:A:H5'   | 1.78                     | 0.83              |
| 51:BS:66:ALA:HA    | 51:BS:69:VAL:HG12 | 1.59                     | 0.83              |
| 55:BW:2:GLU:OE1    | 55:BW:72:LYS:HE3  | 1.77                     | 0.83              |
| 58:BZ:51:ALA:HB1   | 58:BZ:57:ILE:HD11 | 1.58                     | 0.83              |
| 1:AA:1399:C:H5'    | 1:AA:1400:C:H3'   | 1.60                     | 0.83              |
| 3:AC:22:TRP:CE2    | 14:AN:54:PRO:HG2  | 2.13                     | 0.83              |
| 26:B1:11:ARG:HB3   | 26:B1:12:PRO:HD2  | 1.60                     | 0.83              |
| 35:BA:1653:G:H1'   | 35:BA:1654:A:OP2  | 1.78                     | 0.83              |
| 35:BA:2355:C:C2'   | 35:BA:2356:C:H5'  | 2.07                     | 0.83              |
| 35:BA:2358:G:H2'   | 35:BA:2359:C:H5'  | 1.59                     | 0.83              |
| 35:BA:2753:A:HO2'  | 35:BA:2754:U:H5'  | 1.39                     | 0.83              |
| 1:AA:1073:U:O2'    | 1:AA:1074:G:H5'   | 1.77                     | 0.83              |
| 1:AA:63:C:H5'      | 1:AA:64:G:OP2     | 1.78                     | 0.83              |
| 35:BA:108:U:C2'    | 35:BA:109:G:H5'   | 2.08                     | 0.83              |
| 35:BA:1640:C:H2'   | 35:BA:1641:A:H5'  | 1.59                     | 0.83              |
| 35:BA:259:G:H2'    | 35:BA:260:G:H8    | 1.42                     | 0.83              |
| 24:AY:196:ILE:HG13 | 24:AY:197:ARG:H   | 1.43                     | 0.83              |
| 35:BA:71:A:H2      | 56:BX:31:HIS:HE1  | 1.27                     | 0.83              |
| 35:BA:955:C:C2'    | 35:BA:956:G:C5'   | 2.51                     | 0.83              |
| 29:B4:68:ARG:HD3   | 29:B4:71:ARG:HD3  | 1.58                     | 0.83              |
| 31:B6:17:LYS:HA    | 31:B6:17:LYS:HE2  | 1.58                     | 0.83              |
| 35:BA:1038:C:C3'   | 35:BA:1039:G:H5'' | 2.08                     | 0.83              |
| 35:BA:1805:U:C2'   | 35:BA:1806:C:H5'  | 2.08                     | 0.83              |
| 35:BA:2287:A:H62   | 35:BA:2344:U:H3   | 1.27                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2403:C:OP2   | 35:BA:2403:C:C5    | 2.31                     | 0.83              |
| 50:BR:9:LYS:C      | 50:BR:10:LEU:HD23  | 1.99                     | 0.83              |
| 1:AA:1495:U:O2'    | 1:AA:1496:C:H5'    | 1.78                     | 0.83              |
| 1:AA:862:C:H2'     | 1:AA:863:U:C5'     | 2.00                     | 0.83              |
| 2:AB:42:ILE:HD11   | 2:AB:202:PRO:HB2   | 1.60                     | 0.83              |
| 3:AC:152:ILE:HG12  | 3:AC:167:TRP:HB2   | 1.60                     | 0.83              |
| 9:AI:20:ARG:O      | 9:AI:59:PHE:CA     | 2.26                     | 0.83              |
| 25:B0:24:LYS:HB2   | 25:B0:37:LEU:O     | 1.78                     | 0.83              |
| 26:B1:59:THR:O     | 26:B1:60:PHE:CD1   | 2.30                     | 0.83              |
| 35:BA:246:C:C2'    | 35:BA:247:G:C5'    | 2.42                     | 0.83              |
| 37:BC:80:LYS:CE    | 37:BC:120:VAL:HG12 | 2.08                     | 0.83              |
| 42:BH:43:VAL:HG12  | 42:BH:52:VAL:HG22  | 1.59                     | 0.83              |
| 47:BO:107:ARG:HD3  | 52:BT:36:GLU:HG3   | 1.60                     | 0.83              |
| 2:AB:228:GLY:CA    | 2:AB:229:VAL:CB    | 2.56                     | 0.83              |
| 7:AG:121:ALA:N     | 7:AG:124:LEU:HD13  | 1.92                     | 0.83              |
| 13:AM:4:ILE:HG22   | 13:AM:5:ALA:H      | 1.41                     | 0.83              |
| 19:AS:62:ILE:HD13  | 19:AS:62:ILE:O     | 1.78                     | 0.83              |
| 35:BA:1596:A:C2'   | 35:BA:1597:A:C5'   | 2.53                     | 0.83              |
| 35:BA:955:C:O2'    | 35:BA:956:G:H5'    | 1.79                     | 0.83              |
| 46:BN:3:THR:HG22   | 46:BN:4:TYR:H      | 1.43                     | 0.83              |
| 2:AB:16:HIS:CE1    | 2:AB:210:SER:HG    | 1.97                     | 0.83              |
| 10:AJ:58:ASP:O     | 10:AJ:59:SER:HB3   | 1.79                     | 0.83              |
| 14:AN:25:VAL:HG23  | 14:AN:38:GLY:O     | 1.77                     | 0.83              |
| 19:AS:62:ILE:HA    | 19:AS:66:MET:HE2   | 1.59                     | 0.83              |
| 24:AY:99:ARG:HD3   | 24:AY:401:SER:CA   | 2.09                     | 0.83              |
| 29:B4:14:ILE:O     | 29:B4:15:ILE:HD12  | 1.79                     | 0.83              |
| 31:B6:7:ILE:HG21   | 31:B6:27:LYS:HZ2   | 1.38                     | 0.83              |
| 35:BA:953:A:H61    | 35:BA:965:C:N4     | 1.77                     | 0.83              |
| 39:BE:75:VAL:O     | 39:BE:77:ILE:N     | 2.11                     | 0.83              |
| 40:BF:110:LEU:HD22 | 40:BF:202:PHE:HE1  | 1.41                     | 0.83              |
| 41:BG:137:GLU:HG2  | 41:BG:154:GLY:CA   | 2.09                     | 0.83              |
| 26:B1:26:ARG:HG3   | 26:B1:27:GLU:H     | 1.43                     | 0.83              |
| 35:BA:1697:G:H3'   | 35:BA:1698:A:H5'   | 1.59                     | 0.83              |
| 35:BA:523:C:H2'    | 35:BA:524:U:H5'    | 1.58                     | 0.83              |
| 35:BA:833:U:C4'    | 48:BP:52:GLU:H     | 1.91                     | 0.83              |
| 1:AA:1250:A:H4'    | 9:AI:68:GLY:H      | 1.44                     | 0.83              |
| 1:AA:40:C:H2'      | 1:AA:41:G:H8       | 1.44                     | 0.83              |
| 2:AB:152:PHE:CE1   | 2:AB:155:LEU:CD1   | 2.62                     | 0.83              |
| 2:AB:185:ILE:HG23  | 2:AB:199:TYR:HB2   | 1.61                     | 0.83              |
| 9:AI:20:ARG:O      | 9:AI:59:PHE:HB3    | 1.77                     | 0.83              |
| 24:AY:17:ILE:HG22  | 24:AY:25:LYS:HG2   | 1.59                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:B3:7:LYS:HG3    | 28:B3:32:GLN:O     | 1.79                     | 0.83              |
| 35:BA:1291:C:H2'   | 35:BA:1292:U:C6    | 2.14                     | 0.83              |
| 35:BA:2007:C:HO2'  | 35:BA:2008:C:H5'   | 1.40                     | 0.83              |
| 35:BA:2581:G:C6    | 35:BA:2610:C:N3    | 2.47                     | 0.83              |
| 48:BP:52:GLU:HG2   | 48:BP:57:THR:CB    | 2.09                     | 0.83              |
| 2:AB:228:GLY:CA    | 2:AB:229:VAL:CG1   | 2.45                     | 0.82              |
| 35:BA:2010:G:C2'   | 35:BA:2011:U:C5'   | 2.57                     | 0.82              |
| 35:BA:327:G:H2'    | 35:BA:328:U:C6     | 2.14                     | 0.82              |
| 57:BY:81:LYS:HD3   | 57:BY:97:ARG:HG3   | 1.60                     | 0.82              |
| 3:AC:187:ALA:CB    | 3:AC:198:VAL:HB    | 2.09                     | 0.82              |
| 4:AD:148:VAL:HG12  | 4:AD:149:ALA:H     | 1.40                     | 0.82              |
| 9:AI:23:ASN:ND2    | 9:AI:23:ASN:H      | 1.76                     | 0.82              |
| 24:AY:507:TYR:CE1  | 24:AY:572:TYR:HA   | 2.13                     | 0.82              |
| 35:BA:654(N):G:H2' | 35:BA:654(O):G:O4' | 1.77                     | 0.82              |
| 42:BH:168:PRO:CA   | 42:BH:170:ARG:HH22 | 1.93                     | 0.82              |
| 49:BQ:141:GLN:O    | 58:BZ:53:ILE:HB    | 1.79                     | 0.82              |
| 57:BY:28:LYS:HD2   | 57:BY:28:LYS:N     | 1.92                     | 0.82              |
| 1:AA:1129:C:O5'    | 1:AA:1130:A:H5'    | 1.79                     | 0.82              |
| 1:AA:938:A:H2'     | 1:AA:939:G:C5'     | 2.09                     | 0.82              |
| 31:B6:12:GLU:HG3   | 31:B6:23:THR:HG22  | 1.61                     | 0.82              |
| 31:B6:53:LYS:HD3   | 31:B6:54:ILE:H     | 1.43                     | 0.82              |
| 40:BF:6:VAL:HG12   | 40:BF:7:TYR:N      | 1.93                     | 0.82              |
| 42:BH:30:LYS:HE2   | 42:BH:81:GLU:CG    | 2.08                     | 0.82              |
| 1:AA:1049:U:H4'    | 1:AA:1050:G:C5'    | 2.08                     | 0.82              |
| 1:AA:105:G:C5      | 1:AA:106:C:C4      | 2.67                     | 0.82              |
| 1:AA:1399:C:H5'    | 1:AA:1401:G:H5'    | 1.61                     | 0.82              |
| 15:AO:87:ILE:HG22  | 15:AO:88:ARG:N     | 1.94                     | 0.82              |
| 31:B6:12:GLU:CG    | 31:B6:23:THR:HG22  | 2.10                     | 0.82              |
| 38:BD:108:PRO:HG2  | 38:BD:111:LEU:HB2  | 1.60                     | 0.82              |
| 1:AA:1053:G:C4'    | 1:AA:1054:C:H5'    | 2.07                     | 0.82              |
| 25:B0:7:LEU:CD1    | 49:BQ:85:LYS:HE2   | 2.09                     | 0.82              |
| 31:B6:44:ARG:O     | 31:B6:45:LYS:HG2   | 1.79                     | 0.82              |
| 31:B6:41:PRO:CD    | 31:B6:46:HIS:H     | 1.90                     | 0.82              |
| 35:BA:1022:G:N2    | 35:BA:1142(A):A:C2 | 2.47                     | 0.82              |
| 35:BA:2469:A:H2'   | 35:BA:2470:G:H5'   | 1.60                     | 0.82              |
| 46:BN:58:ASP:O     | 46:BN:60:ILE:HG13  | 1.79                     | 0.82              |
| 51:BS:97:ARG:HH21  | 51:BS:98:VAL:CA    | 1.93                     | 0.82              |
| 1:AA:961:U:O2'     | 1:AA:962:C:H5'     | 1.79                     | 0.82              |
| 1:AA:979:C:C2'     | 1:AA:980:C:H5''    | 2.10                     | 0.82              |
| 2:AB:145:LEU:CD2   | 2:AB:149:LEU:CD2   | 2.58                     | 0.82              |
| 2:AB:16:HIS:CE1    | 2:AB:210:SER:OG    | 2.33                     | 0.82              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:AB:75:LYS:HA      | 2:AB:78:GLN:HE21   | 1.44                     | 0.82              |
| 35:BA:2000:G:N2     | 35:BA:2001:A:N9    | 2.28                     | 0.82              |
| 35:BA:2313:C:H4'    | 41:BG:40:ASN:ND2   | 1.95                     | 0.82              |
| 52:BT:106:SER:HA    | 52:BT:110:ILE:HG12 | 1.61                     | 0.82              |
| 54:BV:19:LYS:HG2    | 54:BV:94:LEU:HB2   | 1.61                     | 0.82              |
| 58:BZ:69:THR:HG22   | 58:BZ:90:VAL:HA    | 1.61                     | 0.82              |
| 2:AB:145:LEU:HD22   | 2:AB:149:LEU:HD23  | 1.62                     | 0.82              |
| 14:AN:27:CYS:SG     | 14:AN:29:ARG:HB2   | 2.20                     | 0.82              |
| 1:AA:375:U:OP1      | 16:AP:69:THR:HG21  | 1.79                     | 0.82              |
| 26:B1:57:GLU:O      | 26:B1:58:ILE:HG13  | 1.79                     | 0.82              |
| 35:BA:1747(A):G:H2' | 35:BA:1748:G:C5'   | 2.08                     | 0.82              |
| 50:BR:4:LEU:HG      | 50:BR:4:LEU:O      | 1.77                     | 0.82              |
| 1:AA:792:A:H1'      | 1:AA:793:U:OP2     | 1.79                     | 0.82              |
| 10:AJ:78:ASN:HD22   | 10:AJ:80:LYS:H     | 1.27                     | 0.82              |
| 20:AT:74:LYS:CG     | 20:AT:75:ASN:H     | 1.87                     | 0.82              |
| 27:B2:8:LYS:O       | 27:B2:11:GLU:CG    | 2.28                     | 0.82              |
| 31:B6:33:LYS:HA     | 31:B6:33:LYS:HE2   | 1.59                     | 0.82              |
| 35:BA:2610:C:O2'    | 35:BA:2611:U:P     | 2.38                     | 0.82              |
| 35:BA:702:G:HO2'    | 35:BA:703:U:H5'    | 1.43                     | 0.82              |
| 36:BB:8:U:H5'       | 36:BB:8:U:H6       | 1.43                     | 0.82              |
| 37:BC:54:ARG:NH2    | 37:BC:56:ASP:HB3   | 1.95                     | 0.82              |
| 39:BE:52:LEU:HD11   | 52:BT:1:MET:HE3    | 1.60                     | 0.82              |
| 1:AA:1525:G:C2'     | 1:AA:1526:G:H5'    | 2.10                     | 0.82              |
| 1:AA:198:G:C4       | 1:AA:199:G:N7      | 2.47                     | 0.82              |
| 2:AB:114:ARG:HH12   | 2:AB:118:LEU:HD11  | 1.43                     | 0.82              |
| 33:B8:32:LEU:HD22   | 35:BA:2392:A:OP1   | 1.78                     | 0.82              |
| 35:BA:262:A:C2'     | 35:BA:263:C:H5'    | 2.10                     | 0.82              |
| 35:BA:43:A:H2'      | 35:BA:44:G:H5'     | 1.59                     | 0.82              |
| 35:BA:693:C:H2'     | 35:BA:694:U:H6     | 1.43                     | 0.82              |
| 50:BR:45:ARG:HG3    | 50:BR:46:GLY:N     | 1.95                     | 0.82              |
| 53:BU:92:ARG:NH1    | 53:BU:94:ASN:HD22  | 1.78                     | 0.82              |
| 1:AA:88:A:C4'       | 1:AA:89:C:H5'      | 2.08                     | 0.82              |
| 9:AI:19:LEU:HA      | 9:AI:61:ALA:HB2    | 0.85                     | 0.82              |
| 22:AV:44:G:C2'      | 22:AV:45:U:H5'     | 2.09                     | 0.82              |
| 29:B4:12:ALA:C      | 29:B4:24:THR:HG23  | 1.97                     | 0.82              |
| 35:BA:1798:U:OP2    | 38:BD:274:ARG:NH2  | 2.12                     | 0.82              |
| 35:BA:1820:U:O2'    | 38:BD:201:HIS:HD2  | 1.63                     | 0.82              |
| 38:BD:35:LYS:NZ     | 38:BD:35:LYS:HB3   | 1.93                     | 0.82              |
| 1:AA:346:G:H4'      | 52:BT:41:ARG:NH2   | 1.95                     | 0.81              |
| 20:AT:74:LYS:HG3    | 20:AT:75:ASN:N     | 1.94                     | 0.81              |
| 31:B6:10:LEU:HD22   | 31:B6:10:LEU:N     | 1.94                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2358:G:O2'   | 35:BA:2359:C:H5'   | 1.80                     | 0.81              |
| 1:AA:359:U:HO2'    | 1:AA:360:A:H5'     | 1.41                     | 0.81              |
| 2:AB:128:GLU:HG3   | 2:AB:128:GLU:O     | 1.80                     | 0.81              |
| 27:B2:16:LEU:HD22  | 27:B2:20:GLU:HG3   | 1.60                     | 0.81              |
| 30:B5:53:ALA:HA    | 30:B5:56:LYS:HZ1   | 1.42                     | 0.81              |
| 35:BA:1779:U:C5    | 35:BA:1784:A:N7    | 2.49                     | 0.81              |
| 35:BA:2127:G:C2'   | 35:BA:2128:C:H5'   | 2.10                     | 0.81              |
| 39:BE:69:LYS:HE2   | 39:BE:69:LYS:H     | 1.43                     | 0.81              |
| 35:BA:2415:G:O3'   | 48:BP:66:GLY:HA3   | 1.80                     | 0.81              |
| 52:BT:129:ARG:NH1  | 52:BT:131:ALA:HB3  | 1.95                     | 0.81              |
| 58:BZ:74:VAL:HG22  | 58:BZ:86:VAL:HG13  | 1.62                     | 0.81              |
| 5:AE:68:GLU:HG3    | 5:AE:68:GLU:O      | 1.78                     | 0.81              |
| 30:B5:29:THR:HG21  | 35:BA:2815:C:H5'   | 1.62                     | 0.81              |
| 35:BA:2581:G:H2'   | 35:BA:2610:C:H41   | 1.45                     | 0.81              |
| 35:BA:29:U:C2'     | 35:BA:30:G:H5'     | 2.10                     | 0.81              |
| 52:BT:102:ILE:HB   | 52:BT:110:ILE:HD12 | 1.62                     | 0.81              |
| 1:AA:1442(A):G:O6  | 52:BT:118:ARG:HB2  | 1.80                     | 0.81              |
| 1:AA:697:U:H2'     | 1:AA:698:G:C5'     | 2.10                     | 0.81              |
| 27:B2:47:ASN:ND2   | 35:BA:94(A):G:H21  | 1.78                     | 0.81              |
| 33:B8:32:LEU:HB2   | 33:B8:36:LYS:NZ    | 1.95                     | 0.81              |
| 1:AA:773:G:H2'     | 1:AA:774:G:H8      | 1.45                     | 0.81              |
| 35:BA:896:A:C1'    | 58:BZ:176:PRO:HG3  | 2.10                     | 0.81              |
| 36:BB:56:G:H5'     | 41:BG:27:ASN:HD21  | 1.44                     | 0.81              |
| 37:BC:149:ASN:HD22 | 37:BC:152:GLU:HB3  | 1.46                     | 0.81              |
| 1:AA:1151:A:C4     | 1:AA:1152:A:N7     | 2.49                     | 0.81              |
| 1:AA:115:G:H4'     | 1:AA:116:A:O5'     | 1.80                     | 0.81              |
| 1:AA:771:G:C6      | 1:AA:772:U:O4      | 2.33                     | 0.81              |
| 27:B2:48:HIS:O     | 27:B2:52:ASP:HB2   | 1.81                     | 0.81              |
| 35:BA:2010:G:H2'   | 35:BA:2011:U:C5'   | 2.09                     | 0.81              |
| 29:B4:40:HIS:NE2   | 41:BG:118:ARG:HA   | 1.95                     | 0.81              |
| 47:BO:49:ARG:HA    | 47:BO:53:LYS:HZ1   | 1.46                     | 0.81              |
| 48:BP:47:ASP:HB3   | 48:BP:49:ARG:N     | 1.95                     | 0.81              |
| 55:BW:26:GLY:H     | 55:BW:71:VAL:HG23  | 1.45                     | 0.81              |
| 1:AA:1101:A:H4'    | 1:AA:1102:A:O5'    | 1.81                     | 0.81              |
| 1:AA:347:G:O2'     | 1:AA:348:G:H5''    | 1.80                     | 0.81              |
| 9:AI:20:ARG:O      | 9:AI:59:PHE:HA     | 1.79                     | 0.81              |
| 35:BA:666:G:OP1    | 48:BP:47:ASP:O     | 1.98                     | 0.81              |
| 36:BB:40:U:H3'     | 36:BB:41:U:C5'     | 2.11                     | 0.81              |
| 37:BC:117:THR:HG22 | 37:BC:119:ASP:N    | 1.96                     | 0.81              |
| 1:AA:1307:U:H2'    | 1:AA:1308:U:H6     | 1.44                     | 0.81              |
| 35:BA:1062:G:H1    | 35:BA:1075:C:H42   | 1.27                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BA:1170:G:H1   | 35:BA:1179:C:H42  | 1.28                     | 0.81              |
| 35:BA:2491:U:H5'  | 35:BA:2570:G:H5'' | 1.63                     | 0.81              |
| 36:BB:16:G:HO2'   | 36:BB:17:C:H6     | 1.25                     | 0.81              |
| 2:AB:145:LEU:HD22 | 2:AB:149:LEU:CD2  | 2.11                     | 0.81              |
| 10:AJ:30:SER:OG   | 10:AJ:81:THR:HG22 | 1.81                     | 0.81              |
| 24:AY:572:TYR:HD1 | 24:AY:572:TYR:H   | 1.29                     | 0.81              |
| 26:B1:53:VAL:HG21 | 26:B1:58:ILE:HD12 | 1.63                     | 0.81              |
| 26:B1:75:GLU:O    | 26:B1:78:LYS:HD2  | 1.80                     | 0.81              |
| 35:BA:1273:U:H5'' | 35:BA:1646:C:H42  | 1.44                     | 0.81              |
| 35:BA:459:U:C2'   | 35:BA:460:A:H5'   | 2.10                     | 0.81              |
| 42:BH:10:PRO:HB2  | 42:BH:49:VAL:HG12 | 1.62                     | 0.81              |
| 48:BP:16:ARG:NE   | 48:BP:18:ARG:HG2  | 1.96                     | 0.81              |
| 48:BP:23:PRO:HG2  | 48:BP:33:ARG:HH21 | 1.46                     | 0.81              |
| 1:AA:737:A:H1'    | 6:AF:73:ASN:HD21  | 1.45                     | 0.81              |
| 35:BA:2363:C:HO2' | 35:BA:2364:C:H5'  | 1.43                     | 0.81              |
| 1:AA:1148:U:H2'   | 1:AA:1149:C:H5'   | 1.63                     | 0.81              |
| 1:AA:543:C:C2'    | 1:AA:544:G:C5'    | 2.55                     | 0.81              |
| 2:AB:231:GLU:HB2  | 2:AB:232:PRO:HD3  | 1.60                     | 0.81              |
| 27:B2:64:LEU:HD23 | 27:B2:64:LEU:C    | 2.02                     | 0.81              |
| 35:BA:1983:C:O2'  | 35:BA:1984:G:H5'' | 1.81                     | 0.81              |
| 35:BA:1996:C:H4'  | 35:BA:1997:G:OP1  | 1.81                     | 0.81              |
| 27:B2:10:LEU:HD13 | 35:BA:78:A:OP1    | 1.80                     | 0.81              |
| 38:BD:35:LYS:N    | 38:BD:36:PRO:HD2  | 1.96                     | 0.81              |
| 41:BG:66:GLN:NE2  | 41:BG:94:LEU:HG   | 1.96                     | 0.81              |
| 52:BT:28:VAL:O    | 52:BT:29:ARG:HB2  | 1.81                     | 0.81              |
| 2:AB:89:GLY:C     | 2:AB:90:MET:HG2   | 2.00                     | 0.80              |
| 36:BB:80:U:H2'    | 36:BB:81:G:H21    | 1.43                     | 0.80              |
| 38:BD:30:GLU:HG3  | 38:BD:63:ARG:NE   | 1.94                     | 0.80              |
| 41:BG:41:GLN:OE1  | 41:BG:56:ALA:HB1  | 1.81                     | 0.80              |
| 49:BQ:76:LYS:HB3  | 49:BQ:91:GLU:HG3  | 1.62                     | 0.80              |
| 58:BZ:81:ARG:CZ   | 58:BZ:81:ARG:HB2  | 2.10                     | 0.80              |
| 1:AA:46:G:HO2'    | 1:AA:365:U:H1'    | 1.45                     | 0.80              |
| 22:AV:44:G:H2'    | 22:AV:45:U:H5'    | 1.61                     | 0.80              |
| 35:BA:1999:C:H2'  | 35:BA:2000:G:H5'  | 1.61                     | 0.80              |
| 35:BA:2807:G:H3'  | 35:BA:2808:U:H5'' | 1.62                     | 0.80              |
| 41:BG:102:PHE:O   | 41:BG:106:LEU:HB3 | 1.80                     | 0.80              |
| 1:AA:360:A:C2'    | 1:AA:361:G:H5'    | 2.11                     | 0.80              |
| 1:AA:489:C:O2'    | 1:AA:490:G:H5'    | 1.81                     | 0.80              |
| 1:AA:939:G:H2'    | 1:AA:940:C:C6     | 2.17                     | 0.80              |
| 36:BB:56:G:C5'    | 41:BG:27:ASN:HD21 | 1.95                     | 0.80              |
| 54:BV:15:GLU:CG   | 54:BV:16:PRO:HD2  | 2.11                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1384:C:C2'   | 1:AA:1385:G:H5'   | 2.12                     | 0.80              |
| 1:AA:321:A:O2'    | 1:AA:322:C:H5'    | 1.81                     | 0.80              |
| 1:AA:936:C:C2'    | 1:AA:937:A:H5'    | 2.12                     | 0.80              |
| 2:AB:164:VAL:O    | 2:AB:186:ALA:HA   | 1.81                     | 0.80              |
| 4:AD:101:LEU:HB2  | 4:AD:138:TYR:HB3  | 1.62                     | 0.80              |
| 9:AI:20:ARG:O     | 9:AI:59:PHE:CB    | 2.29                     | 0.80              |
| 33:B8:52:LYS:N    | 33:B8:53:PRO:HD2  | 1.96                     | 0.80              |
| 35:BA:2710:C:HO2' | 35:BA:2711:A:H5'  | 1.45                     | 0.80              |
| 35:BA:1187:G:H5'' | 54:BV:81:TYR:CE2  | 2.16                     | 0.80              |
| 1:AA:198:G:O6     | 1:AA:220:G:C5     | 2.35                     | 0.80              |
| 1:AA:308:C:H2'    | 1:AA:309:G:C8     | 2.15                     | 0.80              |
| 1:AA:490:G:H2'    | 1:AA:491:G:H8     | 1.46                     | 0.80              |
| 35:BA:1021:A:H2'  | 35:BA:1022:G:H4'  | 1.62                     | 0.80              |
| 35:BA:1517:G:H5'  | 35:BA:1517:G:H8   | 1.45                     | 0.80              |
| 35:BA:142:A:H8    | 35:BA:1595:G:H21  | 1.26                     | 0.80              |
| 35:BA:1596:A:H2'  | 35:BA:1597:A:C5'  | 2.09                     | 0.80              |
| 35:BA:179:G:O2'   | 35:BA:180:G:C5'   | 2.30                     | 0.80              |
| 35:BA:1899:G:H21  | 35:BA:1902:C:N4   | 1.79                     | 0.80              |
| 35:BA:2287:A:N6   | 35:BA:2344:U:H3   | 1.80                     | 0.80              |
| 35:BA:361:G:H2'   | 35:BA:362:U:H5''  | 1.61                     | 0.80              |
| 35:BA:1820:U:O4   | 38:BD:160:GLY:O   | 1.99                     | 0.80              |
| 42:BH:3:ARG:CG    | 42:BH:3:ARG:HH11  | 1.94                     | 0.80              |
| 1:AA:1049:U:OP1   | 14:AN:3:ARG:HD3   | 1.81                     | 0.80              |
| 1:AA:198:G:N3     | 1:AA:199:G:N7     | 2.30                     | 0.80              |
| 2:AB:114:ARG:HH11 | 2:AB:114:ARG:HG3  | 1.44                     | 0.80              |
| 35:BA:2124:G:H1   | 35:BA:2174:C:H42  | 1.30                     | 0.80              |
| 35:BA:742:G:O2'   | 35:BA:743:G:C5'   | 2.30                     | 0.80              |
| 35:BA:963:U:O2'   | 35:BA:964:C:C5'   | 2.30                     | 0.80              |
| 42:BH:85:LYS:HE3  | 42:BH:145:ALA:HB1 | 1.63                     | 0.80              |
| 1:AA:545:C:H2'    | 1:AA:546:G:C5'    | 2.02                     | 0.80              |
| 12:AL:27:LEU:HD13 | 12:AL:28:LYS:N    | 1.95                     | 0.80              |
| 34:B9:1:MET:HG2   | 35:BA:2478:A:OP2  | 1.82                     | 0.80              |
| 35:BA:331:A:C1'   | 35:BA:332:A:OP1   | 2.30                     | 0.80              |
| 48:BP:84:ASN:OD1  | 48:BP:116:GLY:HA3 | 1.81                     | 0.80              |
| 1:AA:349:A:O2'    | 1:AA:350:G:C5'    | 2.30                     | 0.80              |
| 4:AD:17:VAL:CG1   | 4:AD:18:LYS:H     | 1.95                     | 0.80              |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CG   | 2.16                     | 0.80              |
| 19:AS:40:ILE:HD11 | 19:AS:62:ILE:CG1  | 2.11                     | 0.80              |
| 29:B4:16:CYS:SG   | 29:B4:19:GLY:O    | 2.39                     | 0.80              |
| 35:BA:1678:G:H22  | 35:BA:1989:G:N2   | 1.62                     | 0.80              |
| 35:BA:1983:C:C2'  | 35:BA:1984:G:C5'  | 2.60                     | 0.80              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BF:154:VAL:HG22 | 40:BF:191:ARG:HB3 | 1.63                     | 0.80              |
| 41:BG:66:GLN:HE22  | 41:BG:94:LEU:HG   | 1.47                     | 0.80              |
| 48:BP:135:LEU:HD21 | 48:BP:144:GLU:HG3 | 1.62                     | 0.80              |
| 48:BP:58:THR:O     | 48:BP:61:ARG:CG   | 2.29                     | 0.80              |
| 1:AA:1176:A:H2'    | 1:AA:1177:G:C8    | 2.17                     | 0.80              |
| 1:AA:197:A:C6      | 1:AA:221:C:C4'    | 2.64                     | 0.80              |
| 1:AA:37:U:O2'      | 1:AA:38:G:C5'     | 2.30                     | 0.80              |
| 24:AY:312:LEU:HD11 | 24:AY:401:SER:HB2 | 1.64                     | 0.80              |
| 35:BA:2131:G:N2    | 35:BA:2133:A:N3   | 2.30                     | 0.80              |
| 29:B4:28:LYS:HD3   | 41:BG:143:GLU:HA  | 1.64                     | 0.80              |
| 48:BP:47:ASP:OD2   | 48:BP:49:ARG:CB   | 2.30                     | 0.80              |
| 53:BU:50:ARG:HH12  | 54:BV:72:VAL:HG12 | 1.46                     | 0.80              |
| 57:BY:26:LYS:HG2   | 57:BY:27:VAL:H    | 1.47                     | 0.80              |
| 1:AA:39:G:C2'      | 1:AA:40:C:H5'     | 2.11                     | 0.80              |
| 1:AA:590:C:HO2'    | 1:AA:591:U:H5'    | 1.46                     | 0.80              |
| 3:AC:123:GLN:NE2   | 3:AC:128:PHE:HB2  | 1.97                     | 0.80              |
| 5:AE:50:GLU:HG3    | 5:AE:52:PRO:HD2   | 1.61                     | 0.80              |
| 1:AA:718:G:H5'     | 11:AK:117:ASN:OD1 | 1.82                     | 0.80              |
| 19:AS:6:LYS:HG3    | 19:AS:7:LYS:H     | 1.46                     | 0.80              |
| 35:BA:1227:G:H2'   | 35:BA:1228:G:H8   | 1.47                     | 0.80              |
| 35:BA:2360:A:O2'   | 35:BA:2361:A:C5'  | 2.30                     | 0.80              |
| 35:BA:83:G:N2      | 35:BA:102:G:H2'   | 1.97                     | 0.80              |
| 39:BE:111:ARG:HA   | 50:BR:2:ARG:HG2   | 1.64                     | 0.80              |
| 48:BP:16:ARG:HD3   | 48:BP:16:ARG:C    | 2.02                     | 0.80              |
| 51:BS:28:VAL:HG12  | 51:BS:29:PHE:H    | 1.47                     | 0.80              |
| 58:BZ:53:ILE:HG22  | 58:BZ:71:VAL:HB   | 1.62                     | 0.80              |
| 1:AA:1027:C:H3'    | 1:AA:1028:C:H5''  | 1.63                     | 0.79              |
| 1:AA:1321:C:H3'    | 1:AA:1322:C:H5''  | 1.64                     | 0.79              |
| 1:AA:773:G:C2      | 1:AA:774:G:C5     | 2.69                     | 0.79              |
| 1:AA:946:A:H2'     | 1:AA:947:G:C8     | 2.17                     | 0.79              |
| 24:AY:171:GLU:HG3  | 24:AY:172:ASP:H   | 1.45                     | 0.79              |
| 35:BA:1210:A:H8    | 35:BA:1210:A:H5'  | 1.47                     | 0.79              |
| 1:AA:198:G:C6      | 1:AA:220:G:N1     | 2.50                     | 0.79              |
| 30:B5:41:PRO:HG2   | 30:B5:44:THR:HG21 | 1.65                     | 0.79              |
| 35:BA:1227:G:O2'   | 35:BA:1228:G:H5'  | 1.83                     | 0.79              |
| 35:BA:16:G:C2'     | 35:BA:17:G:H5'    | 2.12                     | 0.79              |
| 35:BA:1983:C:O2'   | 35:BA:1984:G:C5'  | 2.30                     | 0.79              |
| 41:BG:21:ARG:HE    | 41:BG:21:ARG:HA   | 1.47                     | 0.79              |
| 41:BG:66:GLN:OE1   | 41:BG:94:LEU:HG   | 1.81                     | 0.79              |
| 1:AA:1151:A:C6     | 1:AA:1152:A:N6    | 2.51                     | 0.79              |
| 1:AA:1286:A:O2'    | 1:AA:1287:A:C5'   | 2.30                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:509:A:C5'     | 4:AD:54:TYR:HD2    | 1.94                     | 0.79              |
| 1:AA:685:G:C2'     | 1:AA:686:U:H5'     | 2.12                     | 0.79              |
| 2:AB:187:LEU:HD13  | 2:AB:187:LEU:O     | 1.81                     | 0.79              |
| 2:AB:41:ILE:O      | 2:AB:41:ILE:HG22   | 1.82                     | 0.79              |
| 35:BA:1301:A:H4'   | 35:BA:1302:A:OP1   | 1.81                     | 0.79              |
| 35:BA:967:C:O2'    | 35:BA:968:G:C5'    | 2.30                     | 0.79              |
| 41:BG:21:ARG:NE    | 41:BG:21:ARG:HA    | 1.97                     | 0.79              |
| 54:BV:49:THR:HB    | 54:BV:50:PRO:HD2   | 1.64                     | 0.79              |
| 1:AA:560:U:C4'     | 1:AA:561:U:O5'     | 2.30                     | 0.79              |
| 1:AA:60:A:C1'      | 1:AA:61:G:O4'      | 2.31                     | 0.79              |
| 1:AA:975:A:H8      | 1:AA:975:A:H5'     | 1.47                     | 0.79              |
| 2:AB:230:VAL:HB    | 2:AB:231:GLU:CA    | 2.06                     | 0.79              |
| 2:AB:82:ARG:HH11   | 2:AB:82:ARG:HG3    | 1.46                     | 0.79              |
| 24:AY:21:ILE:H     | 24:AY:21:ILE:HD12  | 1.46                     | 0.79              |
| 25:B0:26:TYR:CE2   | 35:BA:857:C:H1'    | 2.17                     | 0.79              |
| 35:BA:1077:A:C5    | 35:BA:1078:U:H1'   | 2.17                     | 0.79              |
| 35:BA:1381:G:C2'   | 35:BA:1382:G:C5'   | 2.58                     | 0.79              |
| 35:BA:1777:U:O2'   | 35:BA:1778:U:H5'   | 1.82                     | 0.79              |
| 35:BA:2068:U:N3    | 35:BA:2430:A:H2    | 1.78                     | 0.79              |
| 35:BA:327:G:O2'    | 35:BA:328:U:C5'    | 2.30                     | 0.79              |
| 40:BF:20:LEU:HD23  | 40:BF:21:ALA:H     | 1.48                     | 0.79              |
| 41:BG:56:ALA:O     | 41:BG:60:LEU:HB3   | 1.83                     | 0.79              |
| 41:BG:38:VAL:HA    | 41:BG:93:THR:HA    | 1.64                     | 0.79              |
| 58:BZ:28:MET:O     | 58:BZ:34:ASN:HA    | 1.82                     | 0.79              |
| 1:AA:35:G:O2'      | 1:AA:36:C:H5'      | 1.82                     | 0.79              |
| 2:AB:15:VAL:CG1    | 2:AB:15:VAL:O      | 2.30                     | 0.79              |
| 24:AY:614:GLU:HA   | 24:AY:617:MET:HE3  | 1.65                     | 0.79              |
| 33:B8:23:VAL:HG12  | 33:B8:46:ARG:HH11  | 1.45                     | 0.79              |
| 35:BA:1988:C:O2'   | 35:BA:1989:G:C5'   | 2.31                     | 0.79              |
| 35:BA:1992:G:C1'   | 35:BA:1993:U:OP2   | 2.30                     | 0.79              |
| 35:BA:271(P):C:O2' | 35:BA:271(Q):G:H5' | 1.83                     | 0.79              |
| 35:BA:49:A:H4'     | 35:BA:50:U:OP2     | 1.80                     | 0.79              |
| 41:BG:65:GLY:O     | 41:BG:66:GLN:HB3   | 1.81                     | 0.79              |
| 52:BT:93:ARG:HG2   | 52:BT:117:ASP:HA   | 1.63                     | 0.79              |
| 1:AA:1504:G:C4'    | 1:AA:1505:G:OP2    | 2.30                     | 0.79              |
| 1:AA:563:A:H5'     | 1:AA:566:G:N2      | 1.97                     | 0.79              |
| 20:AT:75:ASN:H     | 20:AT:75:ASN:ND2   | 1.79                     | 0.79              |
| 30:B5:57:VAL:HG12  | 30:B5:58:LEU:H     | 1.46                     | 0.79              |
| 35:BA:953:A:O2'    | 35:BA:954:G:C5'    | 2.31                     | 0.79              |
| 35:BA:996:A:H4'    | 53:BU:92:ARG:NE    | 1.96                     | 0.79              |
| 1:AA:106:C:H2'     | 1:AA:107:G:H8      | 1.48                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1282:C:C2'   | 1:AA:1283:G:C5'   | 2.60                     | 0.79              |
| 1:AA:1282:C:H2'   | 1:AA:1283:G:C5'   | 2.13                     | 0.79              |
| 1:AA:1527:C:O2'   | 1:AA:1528:U:H5'   | 1.82                     | 0.79              |
| 1:AA:266:G:C4'    | 1:AA:267:C:O5'    | 2.30                     | 0.79              |
| 35:BA:2127:G:O2'  | 35:BA:2128:C:C5'  | 2.30                     | 0.79              |
| 35:BA:332:A:C1'   | 35:BA:333:G:OP1   | 2.30                     | 0.79              |
| 35:BA:613:G:H5'   | 35:BA:613:G:H8    | 1.45                     | 0.79              |
| 35:BA:692:C:H2'   | 35:BA:693:C:H5'   | 1.63                     | 0.79              |
| 37:BC:20:VAL:O    | 37:BC:21:TYR:HB2  | 1.83                     | 0.79              |
| 40:BF:20:LEU:O    | 40:BF:24:LEU:HD23 | 1.82                     | 0.79              |
| 1:AA:1179:A:HO2'  | 1:AA:1180:A:H5'   | 1.46                     | 0.79              |
| 1:AA:119:A:H4'    | 1:AA:120:A:O5'    | 1.82                     | 0.79              |
| 1:AA:686:U:O2     | 1:AA:704:A:N6     | 2.16                     | 0.79              |
| 1:AA:859:A:H2'    | 1:AA:860:A:H5'    | 1.62                     | 0.79              |
| 13:AM:53:VAL:HG12 | 13:AM:57:ARG:HH21 | 1.48                     | 0.79              |
| 29:B4:35:VAL:HA   | 41:BG:109:VAL:HA  | 1.62                     | 0.79              |
| 35:BA:1820:U:H1'  | 38:BD:202:LYS:HB3 | 1.65                     | 0.79              |
| 35:BA:1769:G:C6   | 35:BA:1984:G:C6   | 2.70                     | 0.79              |
| 35:BA:743:G:O2'   | 35:BA:744:G:C5'   | 2.30                     | 0.79              |
| 40:BF:157:VAL:CG1 | 40:BF:194:MET:HG2 | 2.12                     | 0.79              |
| 42:BH:168:PRO:HA  | 42:BH:170:ARG:NH2 | 1.97                     | 0.79              |
| 1:AA:788:U:C2'    | 1:AA:789:U:H5'    | 2.13                     | 0.79              |
| 4:AD:150:GLU:CD   | 4:AD:151:LYS:H    | 1.85                     | 0.79              |
| 29:B4:12:ALA:N    | 29:B4:24:THR:HG22 | 1.67                     | 0.79              |
| 35:BA:1119:C:O2'  | 35:BA:1120:G:C5'  | 2.31                     | 0.79              |
| 35:BA:1920:C:H5'  | 35:BA:1920:C:H6   | 1.46                     | 0.79              |
| 35:BA:2201:C:C2'  | 35:BA:2202:C:H5'  | 2.13                     | 0.79              |
| 35:BA:38:A:H2'    | 35:BA:39:C:C6     | 2.18                     | 0.79              |
| 35:BA:954:G:O2'   | 35:BA:955:C:C5'   | 2.30                     | 0.79              |
| 35:BA:1819:A:H5'' | 38:BD:158:ALA:HB3 | 1.62                     | 0.79              |
| 1:AA:789:U:H2'    | 1:AA:791:G:OP2    | 1.82                     | 0.79              |
| 35:BA:2033:A:H4'  | 35:BA:2034:U:OP1  | 1.81                     | 0.79              |
| 35:BA:629:G:O6    | 35:BA:634:C:N4    | 2.16                     | 0.79              |
| 36:BB:20:C:C2'    | 36:BB:21:G:H5''   | 2.13                     | 0.79              |
| 1:AA:1150:U:C2'   | 1:AA:1151:A:H5'   | 2.12                     | 0.78              |
| 1:AA:1153:C:O2'   | 1:AA:1154:G:C5'   | 2.30                     | 0.78              |
| 1:AA:115:G:C1'    | 1:AA:116:A:OP2    | 2.30                     | 0.78              |
| 2:AB:114:ARG:NH1  | 2:AB:118:LEU:HD11 | 1.97                     | 0.78              |
| 1:AA:1313:U:C3'   | 19:AS:6:LYS:HZ2   | 1.95                     | 0.78              |
| 35:BA:1596:A:O2'  | 35:BA:1597:A:C5'  | 2.30                     | 0.78              |
| 41:BG:20:ILE:HA   | 41:BG:24:GLY:HA3  | 1.62                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:547:A:C4'     | 1:AA:548:G:O5'     | 2.31                     | 0.78              |
| 5:AE:76:ILE:HG13   | 5:AE:93:PRO:HG3    | 1.66                     | 0.78              |
| 28:B3:19:GLN:HE22  | 28:B3:52:HIS:CE1   | 1.93                     | 0.78              |
| 35:BA:1494:A:H2'   | 35:BA:1495:A:H5''  | 1.63                     | 0.78              |
| 48:BP:112:LEU:H    | 48:BP:128:HIS:CD2  | 2.00                     | 0.78              |
| 48:BP:58:THR:O     | 48:BP:61:ARG:NE    | 2.16                     | 0.78              |
| 50:BR:104:ARG:HG3  | 50:BR:111:LEU:HD11 | 1.64                     | 0.78              |
| 55:BW:9:TYR:H      | 55:BW:102:HIS:HD2  | 1.29                     | 0.78              |
| 58:BZ:151:HIS:CB   | 58:BZ:170:THR:HA   | 2.13                     | 0.78              |
| 58:BZ:115:GLY:N    | 58:BZ:177:PRO:HD3  | 1.98                     | 0.78              |
| 1:AA:1157:A:C1'    | 1:AA:1158:C:OP2    | 2.30                     | 0.78              |
| 1:AA:59:A:H3'      | 1:AA:331:G:H22     | 1.48                     | 0.78              |
| 4:AD:3:ARG:HH21    | 4:AD:5:ILE:HG12    | 1.48                     | 0.78              |
| 24:AY:181:LEU:HD23 | 24:AY:182:ARG:NH1  | 1.97                     | 0.78              |
| 24:AY:100:VAL:HG23 | 24:AY:329:ARG:HB2  | 1.66                     | 0.78              |
| 24:AY:82:ILE:CG2   | 24:AY:82:ILE:O     | 2.32                     | 0.78              |
| 31:B6:12:GLU:HA    | 31:B6:23:THR:HA    | 1.64                     | 0.78              |
| 35:BA:1419:A:O2'   | 35:BA:1420:U:H5''  | 1.82                     | 0.78              |
| 35:BA:1434:A:H61   | 35:BA:1558:A:H62   | 1.30                     | 0.78              |
| 35:BA:2403:C:O2'   | 35:BA:2404:C:H5'   | 1.83                     | 0.78              |
| 54:BV:29:PRO:HA    | 54:BV:61:VAL:HG23  | 1.63                     | 0.78              |
| 12:AL:17:LYS:HD3   | 12:AL:18:VAL:H     | 1.49                     | 0.78              |
| 12:AL:45:PRO:HD3   | 12:AL:51:ALA:O     | 1.83                     | 0.78              |
| 20:AT:26:ASN:HB3   | 20:AT:71:THR:OG1   | 1.84                     | 0.78              |
| 24:AY:165:GLN:HE21 | 24:AY:177:ILE:HG21 | 1.47                     | 0.78              |
| 35:BA:1301:A:N3    | 35:BA:1301:A:H5''  | 1.99                     | 0.78              |
| 35:BA:1475:G:H5'   | 35:BA:1475:G:H8    | 1.48                     | 0.78              |
| 30:B5:2:ALA:HA     | 35:BA:2015:A:C1'   | 2.14                     | 0.78              |
| 35:BA:2126:A:C1'   | 35:BA:2127:G:O4'   | 2.30                     | 0.78              |
| 35:BA:953:A:C2'    | 35:BA:954:G:C5'    | 2.56                     | 0.78              |
| 41:BG:82:LEU:HD13  | 41:BG:88:ILE:HD13  | 1.64                     | 0.78              |
| 35:BA:955:C:OP2    | 49:BQ:14:ARG:HD2   | 1.84                     | 0.78              |
| 1:AA:1029:C:C3'    | 1:AA:1030:C:H5''   | 2.12                     | 0.78              |
| 1:AA:495:A:O2'     | 1:AA:496:A:C2'     | 2.30                     | 0.78              |
| 24:AY:628:ARG:HG2  | 24:AY:628:ARG:HH11 | 1.47                     | 0.78              |
| 24:AY:84:THR:HG23  | 24:AY:85:PRO:HD2   | 1.65                     | 0.78              |
| 33:B8:27:THR:HG23  | 35:BA:2361:A:OP1   | 1.83                     | 0.78              |
| 40:BF:20:LEU:H     | 40:BF:24:LEU:CD2   | 1.97                     | 0.78              |
| 41:BG:117:PHE:HD2  | 41:BG:118:ARG:HD3  | 1.49                     | 0.78              |
| 46:BN:22:THR:HG22  | 46:BN:61:ARG:HD3   | 1.65                     | 0.78              |
| 52:BT:31:SER:N     | 52:BT:43:GLN:O     | 2.16                     | 0.78              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:173:U:C5'    | 1:AA:197:A:H5'     | 2.14                     | 0.78              |
| 2:AB:153:ARG:HG3  | 2:AB:153:ARG:O     | 1.82                     | 0.78              |
| 14:AN:16:PHE:CD1  | 14:AN:16:PHE:N     | 2.51                     | 0.78              |
| 26:B1:3:LYS:HB2   | 26:B1:61:ARG:NH2   | 1.98                     | 0.78              |
| 35:BA:2036:C:O2'  | 35:BA:2037:G:H5'   | 1.83                     | 0.78              |
| 35:BA:691:C:H2'   | 35:BA:692:C:H5'    | 1.66                     | 0.78              |
| 38:BD:24:ILE:CD1  | 38:BD:25:THR:H     | 1.97                     | 0.78              |
| 57:BY:81:LYS:HB3  | 57:BY:96:ILE:HD11  | 1.63                     | 0.78              |
| 24:AY:95:GLU:OE1  | 24:AY:403:GLU:HG2  | 1.83                     | 0.78              |
| 35:BA:1646:C:C5'  | 35:BA:1647:G:H5''  | 2.14                     | 0.78              |
| 35:BA:1887:C:H2'  | 35:BA:1888:G:H5''  | 1.66                     | 0.78              |
| 35:BA:740:U:H2'   | 35:BA:741:G:C8     | 2.18                     | 0.78              |
| 36:BB:3:C:H42     | 36:BB:118:G:H1     | 1.30                     | 0.78              |
| 40:BF:9:ILE:HG12  | 40:BF:14:PRO:CA    | 2.13                     | 0.78              |
| 1:AA:1148:U:O2'   | 1:AA:1149:C:H5'    | 1.84                     | 0.78              |
| 1:AA:155:C:H2'    | 1:AA:156:G:C8      | 2.18                     | 0.78              |
| 1:AA:365:U:C3'    | 1:AA:365:U:O2      | 2.31                     | 0.78              |
| 1:AA:688:G:H2'    | 1:AA:689:C:H6      | 1.48                     | 0.78              |
| 25:B0:42:GLY:O    | 25:B0:57:PHE:CG    | 2.36                     | 0.78              |
| 33:B8:30:ARG:HA   | 33:B8:30:ARG:HE    | 1.48                     | 0.78              |
| 35:BA:1678:G:H22  | 35:BA:1989:G:H22   | 0.79                     | 0.78              |
| 35:BA:2123:G:O2'  | 35:BA:2124:G:H5'   | 1.83                     | 0.78              |
| 41:BG:87:PRO:HG2  | 41:BG:88:ILE:H     | 1.48                     | 0.78              |
| 53:BU:90:VAL:O    | 53:BU:92:ARG:N     | 2.17                     | 0.78              |
| 54:BV:40:LEU:HD22 | 54:BV:46:VAL:HA    | 1.65                     | 0.78              |
| 1:AA:1030:C:H4'   | 1:AA:1030(A):G:H5' | 1.66                     | 0.78              |
| 1:AA:1279:A:C5'   | 1:AA:1280:A:OP1    | 2.32                     | 0.78              |
| 1:AA:311:C:O2'    | 1:AA:312:C:C5'     | 2.32                     | 0.78              |
| 1:AA:688:G:H2'    | 1:AA:689:C:C6      | 2.19                     | 0.78              |
| 2:AB:122:PHE:CE2  | 2:AB:139:LYS:HA    | 2.17                     | 0.78              |
| 3:AC:150:LYS:HE2  | 3:AC:152:ILE:HD11  | 1.65                     | 0.78              |
| 6:AF:69:GLU:O     | 6:AF:72:VAL:HG12   | 1.84                     | 0.78              |
| 41:BG:172:LEU:O   | 41:BG:176:LEU:HB2  | 1.84                     | 0.78              |
| 51:BS:30:ARG:HH11 | 51:BS:97:ARG:HG2   | 1.49                     | 0.78              |
| 1:AA:64:G:C5'     | 1:AA:65:U:OP1      | 2.32                     | 0.78              |
| 2:AB:172:ILE:N    | 2:AB:172:ILE:HD12  | 1.97                     | 0.78              |
| 29:B4:39:CYS:O    | 29:B4:40:HIS:CB    | 2.32                     | 0.78              |
| 35:BA:2206:G:H21  | 35:BA:2207:G:C5'   | 1.88                     | 0.78              |
| 48:BP:46:LYS:HG2  | 48:BP:51:PHE:CD1   | 2.18                     | 0.78              |
| 58:BZ:6:LYS:H     | 58:BZ:6:LYS:HE3    | 1.47                     | 0.78              |
| 1:AA:942:G:C4     | 1:AA:943:U:C5      | 2.72                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:48:LYS:HG2    | 7:AG:49:ILE:HG12   | 1.66                     | 0.77              |
| 28:B3:19:GLN:NE2   | 28:B3:52:HIS:CE1   | 2.49                     | 0.77              |
| 35:BA:1375:C:H2'   | 35:BA:1376:C:H6    | 1.49                     | 0.77              |
| 35:BA:2010:G:O2'   | 35:BA:2011:U:C5'   | 2.30                     | 0.77              |
| 35:BA:2689:U:H5''  | 35:BA:2690:C:H5'   | 1.66                     | 0.77              |
| 41:BG:75:LYS:HG2   | 41:BG:76:SER:H     | 1.46                     | 0.77              |
| 12:AL:41:ARG:HH11  | 12:AL:43:VAL:HG22  | 1.50                     | 0.77              |
| 29:B4:12:ALA:O     | 29:B4:24:THR:HG21  | 1.84                     | 0.77              |
| 35:BA:1375:C:H2'   | 35:BA:1376:C:C6    | 2.19                     | 0.77              |
| 35:BA:49:A:N6      | 35:BA:177:G:C4     | 2.52                     | 0.77              |
| 35:BA:2011:U:O2'   | 35:BA:2012:G:H5'   | 1.83                     | 0.77              |
| 35:BA:2203:U:O3'   | 35:BA:2205:C:P     | 2.42                     | 0.77              |
| 35:BA:2403:C:OP1   | 35:BA:2403:C:C3'   | 2.31                     | 0.77              |
| 39:BE:117:MET:O    | 39:BE:121:ASN:HA   | 1.83                     | 0.77              |
| 52:BT:78:LEU:O     | 52:BT:79:HIS:CD2   | 2.37                     | 0.77              |
| 58:BZ:115:GLY:HA2  | 58:BZ:177:PRO:HD3  | 1.66                     | 0.77              |
| 1:AA:197:A:C5      | 1:AA:221:C:H4'     | 2.17                     | 0.77              |
| 1:AA:633:G:H5'     | 1:AA:634:C:OP2     | 1.83                     | 0.77              |
| 1:AA:685:G:HO2'    | 1:AA:686:U:H5'     | 1.46                     | 0.77              |
| 2:AB:87:ARG:CD     | 2:AB:219:VAL:HG11  | 2.14                     | 0.77              |
| 1:AA:967:C:H4'     | 9:AI:125:TYR:HE1   | 1.48                     | 0.77              |
| 24:AY:264:LEU:HB2  | 61:AY:701:GCP:C6   | 2.14                     | 0.77              |
| 35:BA:1786:A:C1'   | 35:BA:1938:A:N6    | 2.46                     | 0.77              |
| 35:BA:1892:C:HO2'  | 35:BA:1893:C:H5'   | 1.46                     | 0.77              |
| 35:BA:1902:C:H4'   | 38:BD:244:ARG:HA   | 1.65                     | 0.77              |
| 35:BA:1984:G:O2'   | 35:BA:1985:G:C5'   | 2.30                     | 0.77              |
| 35:BA:2713:A:C3'   | 35:BA:2714:G:C5'   | 2.62                     | 0.77              |
| 47:BO:104:ARG:HH12 | 47:BO:107:ARG:NH1  | 1.82                     | 0.77              |
| 52:BT:89:VAL:HB    | 52:BT:91:ARG:HG3   | 1.66                     | 0.77              |
| 1:AA:1502:A:C2     | 1:AA:1505:G:N2     | 2.30                     | 0.77              |
| 2:AB:139:LYS:O     | 2:AB:143:GLU:HG3   | 1.84                     | 0.77              |
| 12:AL:18:VAL:HG23  | 12:AL:19:ARG:N     | 1.99                     | 0.77              |
| 29:B4:1:MET:HB2    | 36:BB:39:A:H61     | 1.50                     | 0.77              |
| 30:B5:16:ARG:HG2   | 30:B5:16:ARG:HH11  | 1.49                     | 0.77              |
| 35:BA:1419:A:O2'   | 35:BA:1421:G:N7    | 2.16                     | 0.77              |
| 35:BA:1640:C:C2'   | 35:BA:1641:A:H5'   | 2.14                     | 0.77              |
| 37:BC:92:ALA:HB2   | 37:BC:154:ILE:HD13 | 1.66                     | 0.77              |
| 42:BH:12:PRO:HD2   | 42:BH:15:VAL:HG21  | 1.66                     | 0.77              |
| 51:BS:97:ARG:HE    | 51:BS:97:ARG:C     | 1.88                     | 0.77              |
| 1:AA:39:G:O2'      | 1:AA:40:C:H5'      | 1.85                     | 0.77              |
| 1:AA:936:C:HO2'    | 1:AA:937:A:H5'     | 1.45                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:936:C:H2'     | 1:AA:937:A:H8      | 1.49                     | 0.77              |
| 35:BA:2715:C:C2'   | 35:BA:2716:U:H5'   | 2.14                     | 0.77              |
| 35:BA:523:C:C2'    | 35:BA:524:U:C5'    | 2.61                     | 0.77              |
| 41:BG:137:GLU:CG   | 41:BG:154:GLY:H    | 1.97                     | 0.77              |
| 48:BP:51:PHE:CD2   | 48:BP:53:GLY:CA    | 2.68                     | 0.77              |
| 7:AG:23:VAL:HG13   | 7:AG:43:PHE:CE2    | 2.19                     | 0.77              |
| 9:AI:11:LYS:O      | 9:AI:12:GLU:HB2    | 1.83                     | 0.77              |
| 13:AM:96:LEU:HB3   | 13:AM:97:PRO:HD2   | 1.66                     | 0.77              |
| 24:AY:584:ILE:HG22 | 24:AY:588:MET:HE2  | 1.67                     | 0.77              |
| 37:BC:24:ASP:O     | 37:BC:28:ARG:HG3   | 1.85                     | 0.77              |
| 48:BP:59:LEU:CA    | 48:BP:61:ARG:HE    | 1.95                     | 0.77              |
| 1:AA:1321:C:H5''   | 1:AA:1322:C:H5''   | 1.64                     | 0.77              |
| 1:AA:918:A:H2'     | 1:AA:919:A:C8      | 2.20                     | 0.77              |
| 2:AB:113:HIS:O     | 2:AB:117:GLU:HG3   | 1.84                     | 0.77              |
| 27:B2:10:LEU:O     | 27:B2:14:ARG:CD    | 2.31                     | 0.77              |
| 29:B4:15:ILE:O     | 29:B4:16:CYS:CB    | 2.31                     | 0.77              |
| 35:BA:146:G:H8     | 35:BA:146:G:H5'    | 1.50                     | 0.77              |
| 35:BA:1799:G:H8    | 38:BD:181:GLU:OE2  | 1.68                     | 0.77              |
| 35:BA:2710:C:O2'   | 35:BA:2711:A:H5'   | 1.84                     | 0.77              |
| 35:BA:605:C:H1'    | 35:BA:657:U:O2'    | 1.85                     | 0.77              |
| 35:BA:654(S):G:H2' | 35:BA:654(T):C:O4' | 1.85                     | 0.77              |
| 35:BA:997:G:OP1    | 53:BU:93:LYS:HD3   | 1.85                     | 0.77              |
| 39:BE:141:ILE:HA   | 39:BE:154:LYS:HE2  | 1.64                     | 0.77              |
| 39:BE:9:VAL:HG23   | 52:BT:4:GLY:HA2    | 1.66                     | 0.77              |
| 1:AA:1071:C:O2'    | 1:AA:1072:G:H5'    | 1.84                     | 0.77              |
| 1:AA:973:G:O4'     | 10:AJ:55:LYS:HG2   | 1.85                     | 0.77              |
| 35:BA:1459:G:N3    | 35:BA:1459:G:H3'   | 1.98                     | 0.77              |
| 35:BA:856:C:H4'    | 35:BA:857:C:OP1    | 1.82                     | 0.77              |
| 37:BC:144:GLY:O    | 37:BC:145:THR:HG23 | 1.85                     | 0.77              |
| 46:BN:133:GLN:HG2  | 46:BN:135:PRO:HD3  | 1.67                     | 0.77              |
| 52:BT:77:PRO:O     | 52:BT:78:LEU:CB    | 2.32                     | 0.77              |
| 1:AA:490:G:C2'     | 1:AA:491:G:H5'     | 2.14                     | 0.77              |
| 3:AC:81:GLY:O      | 3:AC:82:GLU:CG     | 2.31                     | 0.77              |
| 7:AG:15:ASP:O      | 7:AG:19:GLY:HA2    | 1.85                     | 0.77              |
| 12:AL:83:VAL:HG13  | 12:AL:100:ILE:HG23 | 1.67                     | 0.77              |
| 7:AG:81:GLY:HA3    | 23:AX:12:A:H4'     | 1.67                     | 0.77              |
| 35:BA:1653:G:C1'   | 35:BA:1654:A:OP2   | 2.33                     | 0.77              |
| 35:BA:1778:U:HO2'  | 35:BA:1779:U:H5'   | 1.44                     | 0.77              |
| 35:BA:1819:A:H1'   | 35:BA:1820:U:OP2   | 1.85                     | 0.77              |
| 35:BA:2104:G:H1'   | 35:BA:2105:C:OP1   | 1.85                     | 0.77              |
| 35:BA:962:G:C2'    | 35:BA:963:U:H5'    | 2.15                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:607:U:OP1    | 40:BF:103:LYS:HG3  | 1.84                     | 0.77              |
| 44:BK:99:UNK:C     | 44:BK:101:UNK:H    | 1.98                     | 0.77              |
| 48:BP:144:GLU:H    | 48:BP:145:PRO:HD3  | 1.49                     | 0.77              |
| 1:AA:266:G:H5'     | 1:AA:267:C:H5      | 1.36                     | 0.77              |
| 1:AA:494:U:O5'     | 1:AA:494:U:H6      | 1.67                     | 0.77              |
| 24:AY:227:ILE:HG23 | 24:AY:237:PRO:HG2  | 1.65                     | 0.77              |
| 41:BG:38:VAL:HG22  | 41:BG:93:THR:CG2   | 2.08                     | 0.77              |
| 41:BG:61:ALA:HB2   | 41:BG:68:PRO:HD3   | 1.66                     | 0.77              |
| 41:BG:61:ALA:HB1   | 41:BG:67:LYS:HA    | 1.65                     | 0.77              |
| 44:BK:46:UNK:C     | 44:BK:48:UNK:H     | 1.97                     | 0.77              |
| 52:BT:50:ILE:HD11  | 52:BT:102:ILE:HD11 | 1.65                     | 0.77              |
| 58:BZ:165:VAL:HG12 | 58:BZ:166:SER:N    | 1.99                     | 0.77              |
| 1:AA:1306:A:H61    | 1:AA:1331:G:H1'    | 1.49                     | 0.76              |
| 15:AO:28:GLN:O     | 15:AO:32:LEU:HD23  | 1.85                     | 0.76              |
| 22:AV:27:G:H22     | 22:AV:43:C:H5      | 1.32                     | 0.76              |
| 33:B8:62:LEU:HD13  | 35:BA:242:G:C5'    | 2.08                     | 0.76              |
| 35:BA:1799:G:C4'   | 35:BA:1800:C:O5'   | 2.32                     | 0.76              |
| 35:BA:1919:A:H2'   | 35:BA:1920:C:H5''  | 1.66                     | 0.76              |
| 35:BA:743:G:C2'    | 35:BA:744:G:O5'    | 2.33                     | 0.76              |
| 35:BA:195:A:OP1    | 48:BP:46:LYS:NZ    | 2.18                     | 0.76              |
| 48:BP:84:ASN:CG    | 48:BP:116:GLY:CA   | 2.41                     | 0.76              |
| 1:AA:548:G:O2'     | 1:AA:549:C:H5'     | 1.84                     | 0.76              |
| 1:AA:664:G:H22     | 1:AA:741:G:H1      | 1.30                     | 0.76              |
| 20:AT:93:GLU:O     | 20:AT:93:GLU:HG2   | 1.84                     | 0.76              |
| 35:BA:1767:C:O2'   | 35:BA:1768:U:H5'   | 1.86                     | 0.76              |
| 38:BD:35:LYS:H     | 38:BD:36:PRO:HD2   | 1.46                     | 0.76              |
| 39:BE:48:GLN:NE2   | 39:BE:78:LEU:HD22  | 2.00                     | 0.76              |
| 40:BF:2:LYS:HG3    | 40:BF:25:PRO:HG2   | 1.67                     | 0.76              |
| 26:B1:11:ARG:HG2   | 26:B1:11:ARG:HH11  | 1.49                     | 0.76              |
| 35:BA:967:C:O2'    | 35:BA:968:G:H5'    | 1.83                     | 0.76              |
| 41:BG:15:VAL:HG22  | 41:BG:175:LEU:O    | 1.85                     | 0.76              |
| 42:BH:65:HIS:O     | 42:BH:67:LEU:N     | 2.18                     | 0.76              |
| 35:BA:1131:G:H21   | 46:BN:73:THR:HG21  | 1.48                     | 0.76              |
| 2:AB:122:PHE:HE2   | 2:AB:142:LEU:CD2   | 1.95                     | 0.76              |
| 27:B2:8:LYS:HG3    | 27:B2:9:GLN:OE1    | 1.85                     | 0.76              |
| 29:B4:16:CYS:SG    | 29:B4:21:VAL:CG2   | 2.73                     | 0.76              |
| 38:BD:24:ILE:HD13  | 38:BD:25:THR:N     | 2.00                     | 0.76              |
| 40:BF:12:LEU:O     | 40:BF:14:PRO:HD3   | 1.86                     | 0.76              |
| 48:BP:101:VAL:HB   | 48:BP:107:LYS:HA   | 1.67                     | 0.76              |
| 1:AA:1363(A):A:H4' | 1:AA:1364:U:H5''   | 1.68                     | 0.76              |
| 1:AA:1498:U:C1'    | 1:AA:1499:A:OP2    | 2.31                     | 0.76              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:AB:167:PRO:CD    | 2:AB:188:ALA:CB     | 2.58                     | 0.76              |
| 13:AM:108:ARG:HH11 | 13:AM:108:ARG:HG3   | 1.50                     | 0.76              |
| 13:AM:11:ARG:HA    | 13:AM:45:VAL:CB     | 2.12                     | 0.76              |
| 20:AT:74:LYS:CG    | 20:AT:75:ASN:N      | 2.49                     | 0.76              |
| 24:AY:26:THR:HG22  | 24:AY:52:MET:HG2    | 1.67                     | 0.76              |
| 27:B2:69:ARG:O     | 27:B2:70:GLN:CB     | 2.33                     | 0.76              |
| 35:BA:1257:C:O2'   | 40:BF:83:PHE:HA     | 1.84                     | 0.76              |
| 35:BA:17:G:H2'     | 35:BA:18:C:H6       | 1.46                     | 0.76              |
| 35:BA:247:G:H3'    | 35:BA:249:C:C5      | 2.21                     | 0.76              |
| 35:BA:969:U:H2'    | 35:BA:970:C:C6      | 2.21                     | 0.76              |
| 37:BC:27:ALA:O     | 37:BC:30:VAL:HG22   | 1.85                     | 0.76              |
| 40:BF:167:ALA:HB1  | 40:BF:173:VAL:HG11  | 1.68                     | 0.76              |
| 52:BT:60:THR:HG22  | 52:BT:77:PRO:HA     | 1.68                     | 0.76              |
| 35:BA:582:G:OP1    | 53:BU:14:HIS:HD2    | 1.68                     | 0.76              |
| 57:BY:7:VAL:HB     | 57:BY:8:LYS:HZ2     | 1.50                     | 0.76              |
| 1:AA:107:G:H2'     | 1:AA:108:G:O5'      | 1.86                     | 0.76              |
| 1:AA:1384:C:H2'    | 1:AA:1385:G:H5'     | 1.67                     | 0.76              |
| 2:AB:16:HIS:CE1    | 2:AB:210:SER:HA     | 2.21                     | 0.76              |
| 2:AB:91:PRO:HG3    | 2:AB:155:LEU:HD23   | 1.65                     | 0.76              |
| 3:AC:47:LEU:HD23   | 3:AC:68:VAL:HG11    | 1.68                     | 0.76              |
| 35:BA:1087:G:H21   | 35:BA:1103:A:H61    | 1.30                     | 0.76              |
| 35:BA:1019:U:H3    | 35:BA:1142(A):A:H62 | 1.34                     | 0.76              |
| 7:AG:49:ILE:O      | 7:AG:50:ILE:HB      | 1.86                     | 0.76              |
| 22:AV:40:C:H2'     | 22:AV:41:C:H6       | 1.51                     | 0.76              |
| 27:B2:50:ILE:HG22  | 27:B2:51:ARG:N      | 2.00                     | 0.76              |
| 37:BC:153:ILE:HG23 | 37:BC:161:ARG:HH12  | 1.49                     | 0.76              |
| 35:BA:956:G:OP2    | 49:BQ:14:ARG:NH2    | 2.19                     | 0.76              |
| 1:AA:1399:C:C4'    | 1:AA:1400:C:O5'     | 2.31                     | 0.76              |
| 1:AA:1504:G:OP1    | 1:AA:1507:A:H4'     | 1.84                     | 0.76              |
| 2:AB:16:HIS:CE1    | 2:AB:210:SER:O      | 2.39                     | 0.76              |
| 17:AQ:27:PHE:CZ    | 17:AQ:36:ILE:HD11   | 2.20                     | 0.76              |
| 20:AT:26:ASN:HA    | 20:AT:29:LYS:HG3    | 1.68                     | 0.76              |
| 25:B0:10:THR:HG22  | 25:B0:11:ARG:N      | 2.01                     | 0.76              |
| 35:BA:1283:G:N2    | 35:BA:1286:A:OP2    | 2.18                     | 0.76              |
| 35:BA:673:C:H4'    | 40:BF:82:ILE:CD1    | 2.14                     | 0.76              |
| 39:BE:51:PHE:O     | 39:BE:74:PRO:HB2    | 1.86                     | 0.76              |
| 50:BR:58:GLY:HA2   | 50:BR:80:PHE:CE2    | 2.20                     | 0.76              |
| 51:BS:78:LEU:HD11  | 51:BS:103:GLU:CB    | 2.16                     | 0.76              |
| 51:BS:89:ARG:O     | 51:BS:92:TYR:HB3    | 1.85                     | 0.76              |
| 1:AA:859:A:O2'     | 1:AA:860:A:H5'      | 1.86                     | 0.76              |
| 1:AA:940:C:O2'     | 1:AA:941:G:H5'      | 1.86                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:33:TYR:HB3    | 2:AB:41:ILE:O      | 1.85                     | 0.76              |
| 14:AN:12:ARG:C     | 14:AN:14:PRO:HD2   | 2.05                     | 0.76              |
| 31:B6:18:ARG:HG2   | 31:B6:19:ARG:H     | 1.50                     | 0.76              |
| 43:BJ:53:UNK:O     | 43:BJ:85:LEU:HD12  | 1.85                     | 0.76              |
| 1:AA:770:C:O2'     | 1:AA:771:G:C5'     | 2.30                     | 0.76              |
| 3:AC:22:TRP:CZ2    | 14:AN:54:PRO:HG2   | 2.20                     | 0.76              |
| 9:AI:53:VAL:CG1    | 9:AI:95:LYS:HE2    | 2.16                     | 0.76              |
| 39:BE:203:LYS:HE3  | 39:BE:204:ALA:HB2  | 1.65                     | 0.76              |
| 40:BF:80:ALA:HB1   | 40:BF:81:PRO:HD2   | 1.68                     | 0.76              |
| 48:BP:121:LYS:O    | 48:BP:123:LEU:HD23 | 1.85                     | 0.76              |
| 1:AA:265:G:C2'     | 1:AA:266:G:H5''    | 2.11                     | 0.75              |
| 1:AA:696:A:C2'     | 1:AA:697:U:H5'     | 2.16                     | 0.75              |
| 8:AH:42:GLU:HG3    | 8:AH:109:ILE:HD12  | 1.68                     | 0.75              |
| 24:AY:138:LYS:HG2  | 61:AY:701:GCP:C6   | 2.15                     | 0.75              |
| 35:BA:925:C:C2'    | 35:BA:926:A:H5''   | 2.16                     | 0.75              |
| 42:BH:11:VAL:HG23  | 42:BH:50:VAL:HG23  | 1.66                     | 0.75              |
| 58:BZ:165:VAL:HG12 | 58:BZ:166:SER:H    | 1.52                     | 0.75              |
| 1:AA:199:G:O2'     | 1:AA:200:G:H5'     | 1.86                     | 0.75              |
| 3:AC:117:ALA:HB2   | 3:AC:200:ALA:CB    | 2.16                     | 0.75              |
| 35:BA:1676:A:C2    | 35:BA:1993:U:H5'   | 2.20                     | 0.75              |
| 54:BV:19:LYS:HG3   | 54:BV:20:LEU:O     | 1.86                     | 0.75              |
| 1:AA:769:G:O2'     | 1:AA:770:C:H5'     | 1.86                     | 0.75              |
| 13:AM:2:ALA:C      | 13:AM:9:ILE:HG22   | 2.07                     | 0.75              |
| 24:AY:308:PRO:HB2  | 24:AY:394:ALA:HB1  | 1.69                     | 0.75              |
| 35:BA:1215:G:C2'   | 35:BA:1216:G:H5'   | 2.16                     | 0.75              |
| 35:BA:1216:G:C2'   | 35:BA:1217:C:H5'   | 2.17                     | 0.75              |
| 35:BA:1445:A:C8    | 35:BA:1460:A:N1    | 2.54                     | 0.75              |
| 35:BA:407:G:H2'    | 35:BA:408:G:H8     | 1.51                     | 0.75              |
| 35:BA:691:C:C2'    | 35:BA:692:C:H5'    | 2.16                     | 0.75              |
| 39:BE:132:HIS:CA   | 39:BE:135:HIS:CE1  | 2.69                     | 0.75              |
| 39:BE:4:ILE:HD13   | 39:BE:28:ALA:HB1   | 1.67                     | 0.75              |
| 42:BH:156:ALA:O    | 42:BH:158:HIS:HD2  | 1.69                     | 0.75              |
| 52:BT:79:HIS:O     | 52:BT:80:SER:CB    | 2.33                     | 0.75              |
| 52:BT:83:ILE:HG13  | 52:BT:84:GLN:N     | 1.99                     | 0.75              |
| 1:AA:1282:C:O2'    | 1:AA:1283:G:C5'    | 2.34                     | 0.75              |
| 1:AA:342:C:O2'     | 1:AA:343:U:H5'     | 1.86                     | 0.75              |
| 1:AA:495:A:H1'     | 1:AA:496:A:H2'     | 1.69                     | 0.75              |
| 1:AA:687:A:C1'     | 1:AA:688:G:OP2     | 2.30                     | 0.75              |
| 1:AA:973:G:H1'     | 10:AJ:55:LYS:HZ2   | 1.51                     | 0.75              |
| 2:AB:16:HIS:O      | 2:AB:17:PHE:CD1    | 2.40                     | 0.75              |
| 2:AB:190:THR:O     | 2:AB:191:ASP:CB    | 2.35                     | 0.75              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:AO:79:ARG:O    | 15:AO:82:ILE:HG22  | 1.86                     | 0.75              |
| 17:AQ:12:SER:HB3  | 17:AQ:20:THR:HB    | 1.68                     | 0.75              |
| 28:B3:35:ARG:CD   | 28:B3:37:LEU:HD21  | 2.16                     | 0.75              |
| 35:BA:1222:C:H2'  | 35:BA:1223:G:H5'   | 1.66                     | 0.75              |
| 35:BA:661:C:H4'   | 48:BP:16:ARG:HH12  | 1.51                     | 0.75              |
| 37:BC:105:LEU:O   | 37:BC:106:ASP:HB3  | 1.86                     | 0.75              |
| 41:BG:94:LEU:HD12 | 41:BG:98:ARG:CD    | 2.16                     | 0.75              |
| 48:BP:38:GLN:HG3  | 48:BP:39:LYS:H     | 1.51                     | 0.75              |
| 1:AA:1390:U:C2'   | 1:AA:1391:U:H5'    | 2.16                     | 0.75              |
| 2:AB:14:GLY:O     | 2:AB:15:VAL:CG2    | 2.30                     | 0.75              |
| 12:AL:41:ARG:HG2  | 12:AL:42:THR:H     | 1.51                     | 0.75              |
| 19:AS:45:VAL:HB   | 19:AS:64:GLU:HB3   | 1.68                     | 0.75              |
| 35:BA:1722:A:O2'  | 35:BA:1739:U:H5''  | 1.85                     | 0.75              |
| 38:BD:27:THR:CG2  | 38:BD:83:GLU:HG2   | 2.16                     | 0.75              |
| 41:BG:77:ILE:CG1  | 41:BG:82:LEU:HB2   | 2.15                     | 0.75              |
| 35:BA:389:G:H1    | 48:BP:71:VAL:HG12  | 1.51                     | 0.75              |
| 54:BV:64:HIS:ND1  | 54:BV:92:THR:HG22  | 2.01                     | 0.75              |
| 57:BY:95:LYS:HD2  | 57:BY:100:ALA:HA   | 1.69                     | 0.75              |
| 1:AA:521:G:O2'    | 1:AA:522:C:H5'     | 1.87                     | 0.75              |
| 12:AL:6:THR:N     | 12:AL:9:GLN:HE21   | 1.85                     | 0.75              |
| 13:AM:10:PRO:HB2  | 13:AM:18:ALA:HB1   | 1.67                     | 0.75              |
| 13:AM:10:PRO:HB3  | 13:AM:18:ALA:HB1   | 1.69                     | 0.75              |
| 25:B0:37:LEU:H    | 25:B0:37:LEU:HD22  | 1.52                     | 0.75              |
| 35:BA:1396:U:H2'  | 35:BA:1396:U:O2    | 1.86                     | 0.75              |
| 35:BA:1332:G:N2   | 35:BA:1610:A:H8    | 1.83                     | 0.75              |
| 37:BC:102:GLN:C   | 37:BC:104:ILE:H    | 1.89                     | 0.75              |
| 35:BA:2313:C:H4'  | 41:BG:40:ASN:HD21  | 1.52                     | 0.75              |
| 1:AA:37:U:H2'     | 1:AA:38:G:C5'      | 2.12                     | 0.75              |
| 1:AA:949:A:C2'    | 1:AA:950:U:H5'     | 2.07                     | 0.75              |
| 2:AB:172:ILE:H    | 2:AB:172:ILE:CD1   | 1.92                     | 0.75              |
| 24:AY:165:GLN:NE2 | 24:AY:177:ILE:HG21 | 2.01                     | 0.75              |
| 27:B2:2:LYS:HD3   | 27:B2:5:GLU:OE2    | 1.87                     | 0.75              |
| 31:B6:9:LEU:CD1   | 31:B6:9:LEU:O      | 2.31                     | 0.75              |
| 33:B8:61:LEU:HD12 | 33:B8:63:PRO:HD2   | 1.69                     | 0.75              |
| 35:BA:1464:C:H2'  | 35:BA:1465:G:H8    | 1.51                     | 0.75              |
| 35:BA:1770:G:H2'  | 35:BA:1771:C:H5'   | 1.66                     | 0.75              |
| 35:BA:962:G:O2'   | 35:BA:963:U:H5'    | 1.86                     | 0.75              |
| 41:BG:69:ALA:O    | 41:BG:90:LEU:HA    | 1.87                     | 0.75              |
| 49:BQ:141:GLN:C   | 58:BZ:53:ILE:HB    | 2.06                     | 0.75              |
| 1:AA:737:A:H1'    | 6:AF:73:ASN:ND2    | 2.01                     | 0.75              |
| 24:AY:127:LYS:HE3 | 24:AY:128:TYR:HE1  | 1.51                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:55:MET:CG    | 24:AY:56:GLU:N     | 2.32                     | 0.75              |
| 25:B0:19:LYS:HB3   | 25:B0:19:LYS:HZ3   | 1.52                     | 0.75              |
| 27:B2:16:LEU:O     | 27:B2:17:SER:CB    | 2.33                     | 0.75              |
| 35:BA:1417:C:C2'   | 35:BA:1418:G:C5'   | 2.64                     | 0.75              |
| 35:BA:145:G:H2'    | 35:BA:146:G:C5'    | 2.17                     | 0.75              |
| 35:BA:1999:C:O2'   | 35:BA:2000:G:C5'   | 2.30                     | 0.75              |
| 35:BA:246:C:H2'    | 35:BA:247:G:H5'    | 0.82                     | 0.75              |
| 35:BA:599:G:C2'    | 35:BA:600:G:H5'    | 2.16                     | 0.75              |
| 48:BP:124:LYS:HD3  | 48:BP:143:GLY:HA3  | 1.68                     | 0.75              |
| 48:BP:51:PHE:HA    | 48:BP:52:GLU:HB3   | 1.67                     | 0.75              |
| 48:BP:52:GLU:HG2   | 48:BP:57:THR:HB    | 1.68                     | 0.75              |
| 3:AC:83:ARG:O      | 3:AC:86:VAL:HG13   | 1.87                     | 0.75              |
| 22:AV:27:G:H1      | 22:AV:43:C:H41     | 1.35                     | 0.75              |
| 33:B8:32:LEU:HB2   | 33:B8:36:LYS:HZ2   | 1.52                     | 0.75              |
| 35:BA:2245:U:H5'   | 35:BA:2246:G:H5'   | 1.68                     | 0.75              |
| 35:BA:31:C:C2'     | 35:BA:32:C:C5'     | 2.55                     | 0.75              |
| 52:BT:78:LEU:C     | 52:BT:79:HIS:CD2   | 2.60                     | 0.75              |
| 52:BT:96:ARG:HB2   | 52:BT:96:ARG:NH1   | 2.01                     | 0.75              |
| 54:BV:38:LEU:O     | 54:BV:39:LEU:HD13  | 1.86                     | 0.75              |
| 1:AA:359:U:C2'     | 1:AA:360:A:H5'     | 2.17                     | 0.74              |
| 2:AB:187:LEU:O     | 2:AB:187:LEU:CD2   | 2.34                     | 0.74              |
| 9:AI:53:VAL:HG13   | 9:AI:95:LYS:HE2    | 1.69                     | 0.74              |
| 25:B0:27:GLU:CB    | 25:B0:68:GLU:HA    | 2.17                     | 0.74              |
| 35:BA:1809:A:H2'   | 35:BA:1810:A:C8    | 2.21                     | 0.74              |
| 35:BA:2286:A:H4'   | 35:BA:2287:A:O4'   | 1.86                     | 0.74              |
| 37:BC:117:THR:CG2  | 37:BC:119:ASP:N    | 2.50                     | 0.74              |
| 38:BD:65:ILE:HD11  | 38:BD:67:PHE:CE2   | 2.22                     | 0.74              |
| 41:BG:45:GLU:OE2   | 41:BG:152:LEU:HD21 | 1.86                     | 0.74              |
| 41:BG:71:THR:OG1   | 41:BG:89:GLY:HA3   | 1.87                     | 0.74              |
| 1:AA:1229:A:C8     | 1:AA:1229:A:H5'    | 2.20                     | 0.74              |
| 1:AA:771:G:C6      | 1:AA:772:U:C4      | 2.75                     | 0.74              |
| 2:AB:24:TRP:HE3    | 2:AB:32:ILE:HD11   | 1.52                     | 0.74              |
| 13:AM:3:ARG:N      | 13:AM:9:ILE:HG22   | 2.02                     | 0.74              |
| 1:AA:192:U:O4'     | 20:AT:103:GLY:HA2  | 1.87                     | 0.74              |
| 24:AY:157:LEU:HD23 | 24:AY:157:LEU:H    | 1.50                     | 0.74              |
| 31:B6:32:ASN:O     | 31:B6:33:LYS:HG2   | 1.86                     | 0.74              |
| 35:BA:882:G:H2'    | 35:BA:883:G:H8     | 1.52                     | 0.74              |
| 46:BN:128:HIS:HD2  | 46:BN:130:HIS:H    | 1.34                     | 0.74              |
| 48:BP:62:LEU:HD23  | 48:BP:62:LEU:N     | 2.02                     | 0.74              |
| 1:AA:1073:U:H6     | 1:AA:1073:U:O5'    | 1.70                     | 0.74              |
| 1:AA:1371:G:O2'    | 1:AA:1372:U:C5'    | 2.35                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:226:G:O2'    | 1:AA:227:G:H5'     | 1.88                     | 0.74              |
| 1:AA:274:A:O2'    | 1:AA:275:G:O4'     | 2.05                     | 0.74              |
| 1:AA:690:G:C6     | 1:AA:691:G:C6      | 2.75                     | 0.74              |
| 1:AA:770:C:C2'    | 1:AA:771:G:H5'     | 2.17                     | 0.74              |
| 1:AA:774:G:O2'    | 1:AA:775:G:C5'     | 2.30                     | 0.74              |
| 3:AC:81:GLY:C     | 3:AC:82:GLU:CG     | 2.56                     | 0.74              |
| 13:AM:101:GLN:NE2 | 13:AM:101:GLN:H    | 1.86                     | 0.74              |
| 17:AQ:21:VAL:HG21 | 17:AQ:59:ILE:HD11  | 1.68                     | 0.74              |
| 24:AY:290:LYS:O   | 24:AY:400:GLU:HG3  | 1.87                     | 0.74              |
| 30:B5:33:CYS:HB2  | 30:B5:40:LYS:HE3   | 1.68                     | 0.74              |
| 31:B6:15:GLU:CD   | 31:B6:18:ARG:CZ    | 2.55                     | 0.74              |
| 35:BA:1041:G:H22  | 35:BA:1114:G:H22   | 1.31                     | 0.74              |
| 35:BA:673:C:H5''  | 40:BF:81:PRO:HD2   | 1.70                     | 0.74              |
| 35:BA:743:G:C4    | 35:BA:744:G:C8     | 2.75                     | 0.74              |
| 38:BD:35:LYS:N    | 38:BD:36:PRO:CD    | 2.49                     | 0.74              |
| 41:BG:38:VAL:CG2  | 41:BG:93:THR:HG23  | 2.09                     | 0.74              |
| 48:BP:85:LEU:HD23 | 48:BP:86:LYS:N     | 2.02                     | 0.74              |
| 52:BT:27:THR:HG23 | 52:BT:28:VAL:N     | 2.02                     | 0.74              |
| 35:BA:1079:C:O2   | 35:BA:1079:C:H2'   | 1.85                     | 0.74              |
| 35:BA:111:A:O2'   | 35:BA:112:U:C5'    | 2.35                     | 0.74              |
| 35:BA:267:C:H2'   | 35:BA:268:C:H6     | 1.52                     | 0.74              |
| 35:BA:1798:U:H5'  | 38:BD:259:THR:HG22 | 1.69                     | 0.74              |
| 1:AA:105:G:N7     | 1:AA:106:C:N4      | 2.36                     | 0.74              |
| 1:AA:490:G:O2'    | 1:AA:491:G:C5'     | 2.30                     | 0.74              |
| 3:AC:168:ALA:O    | 3:AC:169:ALA:HB2   | 1.86                     | 0.74              |
| 9:AI:53:VAL:HG22  | 9:AI:95:LYS:NZ     | 2.02                     | 0.74              |
| 13:AM:14:ARG:HB3  | 13:AM:16:ASP:OD1   | 1.86                     | 0.74              |
| 35:BA:1332:G:N2   | 35:BA:1610:A:C8    | 2.55                     | 0.74              |
| 38:BD:130:ALA:C   | 38:BD:131:LEU:HD12 | 2.07                     | 0.74              |
| 42:BH:28:GLY:HA3  | 42:BH:79:VAL:HB    | 1.70                     | 0.74              |
| 1:AA:522:C:H2'    | 1:AA:523:A:C5'     | 2.17                     | 0.74              |
| 1:AA:573:A:H8     | 1:AA:573:A:H5'     | 1.52                     | 0.74              |
| 22:AV:47:U:O5'    | 22:AV:47:U:H6      | 1.68                     | 0.74              |
| 26:B1:29:GLY:O    | 26:B1:30:VAL:CG2   | 2.35                     | 0.74              |
| 35:BA:330:A:C2    | 35:BA:1210:A:H2'   | 2.20                     | 0.74              |
| 35:BA:1464:C:O2'  | 35:BA:1465:G:C5'   | 2.30                     | 0.74              |
| 35:BA:1503:U:H2'  | 35:BA:1504:C:C6    | 2.22                     | 0.74              |
| 35:BA:1817:G:C2'  | 35:BA:1818:U:H5'   | 2.17                     | 0.74              |
| 35:BA:628:G:H2'   | 35:BA:629:G:H5''   | 1.70                     | 0.74              |
| 50:BR:56:LYS:HE3  | 50:BR:88:ARG:HA    | 1.69                     | 0.74              |
| 10:AJ:46:ARG:HG2  | 10:AJ:64:GLU:HB3   | 1.70                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B0:50:ASN:HB3   | 25:B0:63:VAL:CG2   | 2.17                     | 0.74              |
| 35:BA:1223:G:N1    | 35:BA:1227:G:C6    | 2.56                     | 0.74              |
| 35:BA:2555:U:C2'   | 35:BA:2556:C:C5'   | 2.49                     | 0.74              |
| 35:BA:2581:G:C2'   | 35:BA:2610:C:H41   | 2.00                     | 0.74              |
| 35:BA:2645:G:H3'   | 35:BA:2646:C:C5'   | 2.15                     | 0.74              |
| 38:BD:176:ARG:HG2  | 38:BD:176:ARG:HH11 | 1.51                     | 0.74              |
| 41:BG:77:ILE:HD12  | 41:BG:80:PHE:HB2   | 1.69                     | 0.74              |
| 56:BX:3:THR:HA     | 56:BX:6:ASP:OD2    | 1.87                     | 0.74              |
| 1:AA:190:U:H3      | 20:AT:105:SER:HB2  | 1.52                     | 0.74              |
| 1:AA:489:C:H2'     | 1:AA:490:G:H8      | 1.53                     | 0.74              |
| 1:AA:509:A:H5'     | 4:AD:54:TYR:CE2    | 2.22                     | 0.74              |
| 35:BA:605:C:H2'    | 35:BA:606:U:H5'    | 1.68                     | 0.74              |
| 42:BH:83:TYR:HB3   | 42:BH:135:GLY:H    | 1.52                     | 0.74              |
| 48:BP:146:VAL:HG22 | 48:BP:147:LEU:N    | 2.02                     | 0.74              |
| 1:AA:186:C:H2'     | 1:AA:187:C:C6      | 2.23                     | 0.74              |
| 1:AA:492:G:O2'     | 1:AA:493:G:H5'     | 1.88                     | 0.74              |
| 1:AA:57:G:O2'      | 1:AA:58:C:H5'      | 1.87                     | 0.74              |
| 12:AL:25:PRO:C     | 12:AL:27:LEU:H     | 1.89                     | 0.74              |
| 20:AT:10:LEU:HD12  | 20:AT:11:SER:H     | 1.51                     | 0.74              |
| 20:AT:16:HIS:O     | 20:AT:19:SER:HB3   | 1.87                     | 0.74              |
| 24:AY:99:ARG:NH2   | 24:AY:403:GLU:HB2  | 2.01                     | 0.74              |
| 27:B2:55:ARG:HG3   | 27:B2:55:ARG:HH11  | 1.52                     | 0.74              |
| 35:BA:1696:G:H2'   | 35:BA:1697:G:H5'   | 1.70                     | 0.74              |
| 35:BA:1970:A:C5'   | 35:BA:1972:A:C1'   | 2.63                     | 0.74              |
| 35:BA:2203:U:HO3'  | 35:BA:2205:C:P     | 2.11                     | 0.74              |
| 27:B2:55:ARG:NH2   | 35:BA:75:G:H4'     | 2.03                     | 0.74              |
| 58:BZ:115:GLY:CA   | 58:BZ:177:PRO:HD3  | 2.16                     | 0.74              |
| 24:AY:631:ILE:HA   | 24:AY:645:ALA:HB2  | 1.69                     | 0.74              |
| 31:B6:12:GLU:HG3   | 31:B6:23:THR:CG2   | 2.18                     | 0.74              |
| 35:BA:1822:G:O2'   | 35:BA:1823:G:C5'   | 2.30                     | 0.74              |
| 35:BA:2403:C:C6    | 35:BA:2403:C:OP2   | 2.41                     | 0.74              |
| 37:BC:48:LEU:HB3   | 37:BC:50:ILE:HD12  | 1.70                     | 0.74              |
| 40:BF:9:ILE:CG1    | 40:BF:14:PRO:HA    | 2.16                     | 0.74              |
| 47:BO:107:ARG:HD3  | 52:BT:36:GLU:CG    | 2.18                     | 0.74              |
| 52:BT:29:ARG:HG2   | 52:BT:86:ILE:HG22  | 1.69                     | 0.74              |
| 53:BU:6:THR:O      | 53:BU:9:VAL:HG22   | 1.86                     | 0.74              |
| 1:AA:198:G:N3      | 1:AA:199:G:C8      | 2.56                     | 0.73              |
| 1:AA:556:C:O2'     | 1:AA:557:G:C5'     | 2.30                     | 0.73              |
| 2:AB:187:LEU:CD2   | 2:AB:201:ILE:O     | 2.30                     | 0.73              |
| 14:AN:16:PHE:HD1   | 14:AN:16:PHE:H     | 1.36                     | 0.73              |
| 24:AY:69:VAL:CA    | 24:AY:82:ILE:HG12  | 2.17                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:1416:G:N3   | 35:BA:1417:C:C4    | 2.55                     | 0.73              |
| 35:BA:2555:U:H2'  | 35:BA:2556:C:H5'   | 0.76                     | 0.73              |
| 1:AA:1193:G:O2'   | 1:AA:1194:U:H5'    | 1.89                     | 0.73              |
| 1:AA:688:G:C6     | 1:AA:700:G:C2      | 2.75                     | 0.73              |
| 1:AA:1190:G:OP1   | 3:AC:4:LYS:HA      | 1.89                     | 0.73              |
| 27:B2:9:GLN:N     | 27:B2:9:GLN:CD     | 2.30                     | 0.73              |
| 29:B4:16:CYS:HA   | 29:B4:33:VAL:HG11  | 1.70                     | 0.73              |
| 35:BA:1041:G:H1   | 35:BA:1114:G:H1    | 1.35                     | 0.73              |
| 35:BA:332:A:C4    | 35:BA:335:C:N4     | 2.55                     | 0.73              |
| 35:BA:523:C:H2'   | 35:BA:524:U:C5'    | 2.17                     | 0.73              |
| 36:BB:43:C:O2'    | 41:BG:94:LEU:HD13  | 1.88                     | 0.73              |
| 52:BT:62:THR:HG22 | 52:BT:75:ILE:HG12  | 1.69                     | 0.73              |
| 52:BT:80:SER:CB   | 52:BT:81:PRO:HD2   | 2.09                     | 0.73              |
| 1:AA:243:A:H4'    | 1:AA:244:U:O5'     | 1.89                     | 0.73              |
| 3:AC:50:ALA:HB2   | 3:AC:75:VAL:CG1    | 2.18                     | 0.73              |
| 35:BA:1036:G:C6   | 35:BA:1120:G:O6    | 2.41                     | 0.73              |
| 35:BA:1423:G:C2'  | 35:BA:1424:G:H5'   | 2.18                     | 0.73              |
| 35:BA:1494:A:N3   | 35:BA:1494:A:H5'   | 2.04                     | 0.73              |
| 35:BA:1819:A:H4'  | 35:BA:1820:U:O5'   | 1.87                     | 0.73              |
| 35:BA:1945:G:C6   | 35:BA:1946:U:C4    | 2.76                     | 0.73              |
| 35:BA:880:G:H2'   | 35:BA:881:G:H5''   | 1.69                     | 0.73              |
| 51:BS:97:ARG:NH2  | 51:BS:98:VAL:HA    | 1.97                     | 0.73              |
| 1:AA:1150:U:H6    | 1:AA:1150:U:O5'    | 1.71                     | 0.73              |
| 1:AA:1277:C:O2'   | 1:AA:1279:A:C8     | 2.22                     | 0.73              |
| 1:AA:950:U:C2'    | 1:AA:951:G:C5'     | 2.30                     | 0.73              |
| 2:AB:130:ARG:NH2  | 2:AB:134:GLU:HG3   | 2.02                     | 0.73              |
| 3:AC:148:GLY:HA2  | 3:AC:171:GLY:HA3   | 1.69                     | 0.73              |
| 3:AC:82:GLU:O     | 3:AC:84:ILE:HG22   | 1.88                     | 0.73              |
| 10:AJ:78:ASN:HD21 | 10:AJ:80:LYS:HB2   | 1.51                     | 0.73              |
| 20:AT:50:GLU:OE2  | 20:AT:100:ILE:HD13 | 1.87                     | 0.73              |
| 29:B4:21:VAL:HG21 | 29:B4:35:VAL:CG2   | 2.18                     | 0.73              |
| 34:B9:17:ILE:HG22 | 34:B9:18:ARG:H     | 1.52                     | 0.73              |
| 35:BA:1041:G:H22  | 35:BA:1114:G:N2    | 1.85                     | 0.73              |
| 35:BA:2152:G:H5'  | 35:BA:2153:G:OP2   | 1.88                     | 0.73              |
| 35:BA:2201:C:H2'  | 35:BA:2202:C:C6    | 2.24                     | 0.73              |
| 35:BA:2751:G:C4   | 42:BH:2:SER:OG     | 2.38                     | 0.73              |
| 42:BH:156:ALA:O   | 42:BH:158:HIS:N    | 2.21                     | 0.73              |
| 1:AA:1255:G:C6    | 1:AA:1283:G:C6     | 2.75                     | 0.73              |
| 1:AA:1402:C:H2'   | 1:AA:1403:C:H5'    | 1.70                     | 0.73              |
| 7:AG:48:LYS:HE2   | 7:AG:115:ARG:HH12  | 1.52                     | 0.73              |
| 9:AI:83:ARG:O     | 9:AI:86:VAL:HG12   | 1.87                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:20:LYS:HD3   | 12:AL:20:LYS:H     | 1.54                     | 0.73              |
| 22:AV:76:A:H4'     | 22:AV:76:A:OP1     | 1.87                     | 0.73              |
| 35:BA:1543:C:H3'   | 35:BA:1544:A:H5''  | 1.70                     | 0.73              |
| 35:BA:2128:C:O2'   | 35:BA:2129:C:C5'   | 2.36                     | 0.73              |
| 35:BA:2606:C:O2'   | 35:BA:2607:G:H5''  | 1.88                     | 0.73              |
| 40:BF:64:ILE:N     | 40:BF:76:GLY:O     | 2.21                     | 0.73              |
| 1:AA:254:G:OP1     | 17:AQ:67:LYS:O     | 2.07                     | 0.73              |
| 24:AY:680:PRO:HD2  | 24:AY:683:VAL:HG21 | 1.70                     | 0.73              |
| 27:B2:17:SER:HB2   | 27:B2:18:PRO:HD2   | 1.70                     | 0.73              |
| 27:B2:70:GLN:CG    | 27:B2:71:ASN:N     | 2.35                     | 0.73              |
| 29:B4:33:VAL:HG13  | 29:B4:34:GLU:H     | 1.52                     | 0.73              |
| 35:BA:1702:G:H2'   | 35:BA:1703:G:O4'   | 1.89                     | 0.73              |
| 35:BA:2126:A:C4'   | 35:BA:2127:G:O5'   | 2.35                     | 0.73              |
| 29:B4:5:ILE:HG21   | 41:BG:67:LYS:HD3   | 1.71                     | 0.73              |
| 3:AC:173:VAL:O     | 3:AC:175:LEU:HD22  | 1.87                     | 0.73              |
| 3:AC:50:ALA:HB2    | 3:AC:75:VAL:HB     | 1.71                     | 0.73              |
| 5:AE:51:VAL:HB     | 5:AE:52:PRO:HD3    | 1.70                     | 0.73              |
| 12:AL:40:VAL:O     | 12:AL:40:VAL:HG12  | 1.88                     | 0.73              |
| 24:AY:126:GLU:HG2  | 24:AY:132:ARG:HH22 | 1.54                     | 0.73              |
| 28:B3:17:LYS:HG2   | 35:BA:969:U:OP1    | 1.88                     | 0.73              |
| 35:BA:1899:G:N2    | 35:BA:1902:C:N4    | 2.35                     | 0.73              |
| 35:BA:2208:A:H1'   | 35:BA:2219:G:C5    | 2.22                     | 0.73              |
| 38:BD:43:ARG:HD2   | 38:BD:44:ASN:OD1   | 1.88                     | 0.73              |
| 42:BH:5:GLY:H      | 42:BH:69:ARG:HD3   | 1.54                     | 0.73              |
| 48:BP:96:THR:HG22  | 48:BP:126:VAL:HB   | 1.69                     | 0.73              |
| 58:BZ:17:ALA:HA    | 58:BZ:20:ARG:CD    | 2.18                     | 0.73              |
| 1:AA:1238:A:OP1    | 1:AA:1335:C:O4'    | 2.06                     | 0.73              |
| 1:AA:1490:C:C2'    | 1:AA:1491:G:C5'    | 2.64                     | 0.73              |
| 1:AA:1504:G:H4'    | 1:AA:1505:G:OP2    | 1.87                     | 0.73              |
| 2:AB:60:ASP:O      | 2:AB:64:ARG:HG2    | 1.89                     | 0.73              |
| 9:AI:18:PHE:O      | 9:AI:61:ALA:HA     | 1.88                     | 0.73              |
| 12:AL:45:PRO:CD    | 12:AL:51:ALA:O     | 2.37                     | 0.73              |
| 20:AT:23:ARG:O     | 20:AT:27:LYS:HB2   | 1.89                     | 0.73              |
| 35:BA:1695:G:H3'   | 35:BA:1695:G:N3    | 2.04                     | 0.73              |
| 40:BF:8:GLN:HB3    | 40:BF:126:VAL:HA   | 1.70                     | 0.73              |
| 42:BH:85:LYS:HZ3   | 42:BH:87:LEU:HG    | 1.54                     | 0.73              |
| 49:BQ:32:TYR:O     | 49:BQ:105:GLU:HB2  | 1.89                     | 0.73              |
| 52:BT:83:ILE:CG1   | 52:BT:84:GLN:N     | 2.52                     | 0.73              |
| 1:AA:311:C:O2'     | 1:AA:312:C:H5'     | 1.87                     | 0.73              |
| 1:AA:938:A:C2'     | 1:AA:939:G:C5'     | 2.64                     | 0.73              |
| 24:AY:168:ILE:HG23 | 24:AY:205:TYR:HE2  | 1.54                     | 0.73              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 24:AY:205:TYR:O     | 24:AY:207:ASP:N    | 2.22                     | 0.73              |
| 24:AY:69:VAL:CB     | 24:AY:82:ILE:HD11  | 2.11                     | 0.73              |
| 33:B8:50:LEU:HD12   | 33:B8:51:ALA:H     | 1.53                     | 0.73              |
| 35:BA:1448:G:H1'    | 35:BA:1528:A:H62   | 1.54                     | 0.73              |
| 35:BA:1653:G:H4'    | 35:BA:1654:A:O5'   | 1.87                     | 0.73              |
| 35:BA:1778:U:O2'    | 35:BA:1779:U:C5'   | 2.31                     | 0.73              |
| 35:BA:1799:G:H3'    | 35:BA:1799:G:P     | 2.29                     | 0.73              |
| 35:BA:2401:U:C2'    | 35:BA:2402:C:OP1   | 2.36                     | 0.73              |
| 35:BA:654(A):G:C2'  | 35:BA:654(B):C:H5' | 2.19                     | 0.73              |
| 38:BD:131:LEU:HB2   | 38:BD:136:ILE:HD11 | 1.69                     | 0.73              |
| 48:BP:64:LYS:O      | 48:BP:66:GLY:N     | 2.22                     | 0.73              |
| 51:BS:17:ARG:O      | 51:BS:20:ARG:HB2   | 1.89                     | 0.73              |
| 1:AA:1179:A:C2'     | 1:AA:1180:A:H5'    | 2.19                     | 0.73              |
| 1:AA:922:G:C6       | 1:AA:923:A:C6      | 2.77                     | 0.73              |
| 18:AR:36:ASN:ND2    | 18:AR:39:VAL:HG23  | 2.03                     | 0.73              |
| 35:BA:1464:C:H2'    | 35:BA:1465:G:C8    | 2.24                     | 0.73              |
| 35:BA:2192:G:O2'    | 35:BA:2193:G:H5''  | 1.89                     | 0.73              |
| 35:BA:2712:U:H1'    | 35:BA:2712(A):A:C8 | 2.23                     | 0.73              |
| 41:BG:77:ILE:HG22   | 41:BG:78:SER:N     | 2.04                     | 0.73              |
| 1:AA:322:C:C2'      | 1:AA:323:U:H5'     | 2.19                     | 0.72              |
| 1:AA:40:C:H2'       | 1:AA:41:G:C8       | 2.23                     | 0.72              |
| 1:AA:555:C:H2'      | 1:AA:556:C:C6      | 2.24                     | 0.72              |
| 24:AY:71:THR:HG21   | 24:AY:357:ARG:HD3  | 1.70                     | 0.72              |
| 35:BA:1291:C:H2'    | 35:BA:1292:U:H6    | 1.53                     | 0.72              |
| 35:BA:1403:C:H5''   | 35:BA:1471:A:H1'   | 1.69                     | 0.72              |
| 35:BA:1819:A:C1'    | 35:BA:1820:U:OP2   | 2.37                     | 0.72              |
| 35:BA:327:G:H2'     | 35:BA:328:U:H6     | 1.51                     | 0.72              |
| 36:BB:80:U:O2'      | 36:BB:81:G:H5''    | 1.88                     | 0.72              |
| 37:BC:117:THR:HG22  | 37:BC:119:ASP:HB2  | 1.69                     | 0.72              |
| 35:BA:2129:C:OP1    | 37:BC:7:ARG:HD2    | 1.89                     | 0.72              |
| 38:BD:44:ASN:CB     | 38:BD:49:ILE:HA    | 2.18                     | 0.72              |
| 39:BE:132:HIS:CD2   | 39:BE:135:HIS:CE1  | 2.77                     | 0.72              |
| 1:AA:1074:G:H2'     | 1:AA:1075:C:C6     | 2.24                     | 0.72              |
| 1:AA:556:C:C2'      | 1:AA:557:G:C5'     | 2.64                     | 0.72              |
| 9:AI:23:ASN:HD22    | 9:AI:23:ASN:H      | 1.32                     | 0.72              |
| 35:BA:1799:G:N2     | 35:BA:1800:C:C5    | 2.57                     | 0.72              |
| 35:BA:2007:C:O2'    | 35:BA:2008:C:C5'   | 2.30                     | 0.72              |
| 35:BA:2103:C:C2'    | 35:BA:2104:G:H5'   | 2.19                     | 0.72              |
| 35:BA:2463:C:O2'    | 35:BA:2464:C:H5'   | 1.87                     | 0.72              |
| 35:BA:2801(A):A:H4' | 35:BA:2802:G:H5'   | 1.71                     | 0.72              |
| 38:BD:79:VAL:HG21   | 38:BD:111:LEU:HD11 | 1.70                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:77:ILE:HB    | 41:BG:82:LEU:O     | 1.88                     | 0.72              |
| 46:BN:96:GLU:O     | 46:BN:100:GLU:HG3  | 1.88                     | 0.72              |
| 49:BQ:12:GLN:HG2   | 49:BQ:73:PRO:HD2   | 1.71                     | 0.72              |
| 52:BT:29:ARG:C     | 52:BT:30:VAL:CG2   | 2.58                     | 0.72              |
| 1:AA:1075:C:O5'    | 1:AA:1075:C:H6     | 1.72                     | 0.72              |
| 1:AA:545:C:C2'     | 1:AA:546:G:C5'     | 2.56                     | 0.72              |
| 6:AF:28:ARG:O      | 6:AF:32:ASN:HB2    | 1.88                     | 0.72              |
| 6:AF:68:PRO:HG2    | 6:AF:71:ARG:HG3    | 1.70                     | 0.72              |
| 7:AG:49:ILE:CD1    | 7:AG:118:VAL:HA    | 2.18                     | 0.72              |
| 7:AG:80:VAL:HB     | 7:AG:83:ALA:HB3    | 1.68                     | 0.72              |
| 10:AJ:8:LEU:HB3    | 10:AJ:96:ILE:HG22  | 1.70                     | 0.72              |
| 25:B0:27:GLU:HB3   | 25:B0:68:GLU:HA    | 1.70                     | 0.72              |
| 27:B2:63:VAL:O     | 27:B2:66:GLU:HG2   | 1.89                     | 0.72              |
| 29:B4:16:CYS:CA    | 29:B4:33:VAL:HG21  | 2.18                     | 0.72              |
| 35:BA:31:C:H6      | 35:BA:31:C:O5'     | 1.72                     | 0.72              |
| 38:BD:30:GLU:CD    | 38:BD:63:ARG:HE    | 1.92                     | 0.72              |
| 1:AA:346:G:H4'     | 52:BT:41:ARG:CZ    | 2.18                     | 0.72              |
| 57:BY:95:LYS:NZ    | 57:BY:99:CYS:O     | 2.22                     | 0.72              |
| 1:AA:1030(B):C:H2' | 1:AA:1030(C):G:C4' | 2.18                     | 0.72              |
| 1:AA:839:U:O2      | 1:AA:839:U:H2'     | 1.89                     | 0.72              |
| 1:AA:89:C:O2'      | 1:AA:90:U:H2'      | 1.89                     | 0.72              |
| 1:AA:1060:C:C5     | 3:AC:2:GLY:HA2     | 2.25                     | 0.72              |
| 8:AH:83:ILE:HD12   | 8:AH:137:VAL:HG22  | 1.71                     | 0.72              |
| 9:AI:104:ARG:C     | 9:AI:104:ARG:HD3   | 2.10                     | 0.72              |
| 24:AY:57:GLN:O     | 24:AY:60:GLU:N     | 2.20                     | 0.72              |
| 24:AY:14:ASN:HD21  | 24:AY:80:ASN:HD22  | 1.36                     | 0.72              |
| 19:AS:64:GLU:HB2   | 29:B4:48:ARG:HH22  | 1.53                     | 0.72              |
| 35:BA:1796:U:H2'   | 35:BA:1797:C:C6    | 2.25                     | 0.72              |
| 1:AA:1151:A:C2     | 1:AA:1152:A:C5     | 2.78                     | 0.72              |
| 1:AA:266:G:O2'     | 1:AA:267:C:C5'     | 2.37                     | 0.72              |
| 1:AA:46:G:H2'      | 1:AA:366:C:N4      | 2.04                     | 0.72              |
| 1:AA:961:U:C1'     | 1:AA:962:C:H5'     | 2.20                     | 0.72              |
| 8:AH:23:SER:HA     | 8:AH:63:LEU:HD22   | 1.71                     | 0.72              |
| 35:BA:1805:U:H5''  | 38:BD:250:TRP:CE2  | 2.25                     | 0.72              |
| 35:BA:2123:G:C2'   | 35:BA:2124:G:H5'   | 2.19                     | 0.72              |
| 35:BA:2023:G:H5'   | 35:BA:2617:C:H4'   | 1.70                     | 0.72              |
| 35:BA:267:C:H2'    | 35:BA:268:C:C6     | 2.24                     | 0.72              |
| 35:BA:2811:G:OP1   | 39:BE:60:ASN:HB2   | 1.90                     | 0.72              |
| 40:BF:24:LEU:O     | 40:BF:26:ALA:N     | 2.21                     | 0.72              |
| 47:BO:35:VAL:HG11  | 47:BO:103:ALA:HB3  | 1.71                     | 0.72              |
| 58:BZ:128:VAL:HG22 | 58:BZ:129:SER:N    | 2.01                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1303:C:C2'    | 1:AA:1304:G:H5'    | 2.19                     | 0.72              |
| 1:AA:1386:G:N2     | 1:AA:1387:G:C5     | 2.57                     | 0.72              |
| 12:AL:47:LYS:N     | 12:AL:48:PRO:HD2   | 2.02                     | 0.72              |
| 24:AY:252:ASP:O    | 24:AY:254:LYS:HE3  | 1.89                     | 0.72              |
| 24:AY:608:VAL:HG22 | 24:AY:671:MET:HB2  | 1.70                     | 0.72              |
| 28:B3:22:ALA:HA    | 28:B3:46:ASN:HD22  | 1.55                     | 0.72              |
| 35:BA:1464:C:HO2'  | 35:BA:1528:A:H8    | 1.36                     | 0.72              |
| 35:BA:654(H):G:C2' | 35:BA:654(I):C:H5' | 2.16                     | 0.72              |
| 52:BT:16:ARG:HG2   | 52:BT:79:HIS:HB3   | 1.71                     | 0.72              |
| 2:AB:192:SER:O     | 2:AB:194:PRO:HD3   | 1.90                     | 0.72              |
| 9:AI:49:PRO:HG2    | 9:AI:81:ILE:HG21   | 1.70                     | 0.72              |
| 25:B0:42:GLY:O     | 25:B0:57:PHE:CD2   | 2.43                     | 0.72              |
| 35:BA:2443:C:O2'   | 35:BA:2444:G:H5'   | 1.89                     | 0.72              |
| 35:BA:2716:U:H2'   | 35:BA:2717:G:H5'   | 1.71                     | 0.72              |
| 35:BA:2807:G:C3'   | 35:BA:2808:U:H5''  | 2.19                     | 0.72              |
| 35:BA:31:C:H2'     | 35:BA:32:C:H5'     | 1.72                     | 0.72              |
| 36:BB:7:G:C2'      | 36:BB:8:U:H5''     | 2.20                     | 0.72              |
| 39:BE:203:LYS:O    | 39:BE:203:LYS:HD2  | 1.90                     | 0.72              |
| 41:BG:55:LYS:O     | 41:BG:59:GLU:HG2   | 1.90                     | 0.72              |
| 42:BH:149:ARG:HD3  | 42:BH:164:TYR:CE1  | 2.25                     | 0.72              |
| 58:BZ:183:LEU:C    | 58:BZ:183:LEU:CD1  | 2.57                     | 0.72              |
| 1:AA:543:C:O2'     | 1:AA:544:G:H5'     | 1.88                     | 0.72              |
| 1:AA:590:C:C2'     | 1:AA:591:U:H5'     | 2.19                     | 0.72              |
| 1:AA:685:G:O2'     | 1:AA:686:U:C5'     | 2.31                     | 0.72              |
| 2:AB:15:VAL:HG21   | 2:AB:209:ARG:NH2   | 2.03                     | 0.72              |
| 3:AC:117:ALA:HB2   | 3:AC:200:ALA:HB2   | 1.72                     | 0.72              |
| 9:AI:26:VAL:HG21   | 9:AI:61:ALA:C      | 2.10                     | 0.72              |
| 19:AS:7:LYS:HD3    | 19:AS:7:LYS:H      | 1.55                     | 0.72              |
| 35:BA:115:C:O2'    | 35:BA:116:C:H5'    | 1.90                     | 0.72              |
| 35:BA:1417:C:H2'   | 35:BA:1418:G:C5'   | 2.20                     | 0.72              |
| 41:BG:60:LEU:O     | 41:BG:63:ILE:HG12  | 1.90                     | 0.72              |
| 1:AA:311:C:H6      | 1:AA:311:C:O5'     | 1.72                     | 0.72              |
| 29:B4:56:VAL:HG23  | 29:B4:60:GLN:HG3   | 1.71                     | 0.72              |
| 35:BA:462:C:HO2'   | 35:BA:463:G:H5'    | 1.54                     | 0.72              |
| 48:BP:51:PHE:HA    | 48:BP:52:GLU:HB2   | 1.70                     | 0.72              |
| 1:AA:118:U:H6      | 1:AA:118:U:O5'     | 1.73                     | 0.72              |
| 1:AA:1280:A:O4'    | 10:AJ:41:PRO:HG3   | 1.90                     | 0.72              |
| 1:AA:356:A:O2'     | 1:AA:368:U:O2'     | 2.03                     | 0.72              |
| 26:B1:75:GLU:O     | 26:B1:78:LYS:CG    | 2.37                     | 0.72              |
| 29:B4:2:LYS:HE2    | 29:B4:4:GLY:O      | 1.89                     | 0.72              |
| 35:BA:1133:U:O3'   | 35:BA:1135:C:P     | 2.48                     | 0.72              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:1658:C:OP1   | 39:BE:132:HIS:O   | 2.07                     | 0.72              |
| 35:BA:2206:G:H3'   | 35:BA:2206:G:N3   | 2.05                     | 0.72              |
| 37:BC:88:GLU:CB    | 37:BC:92:ALA:HB3  | 2.19                     | 0.72              |
| 42:BH:158:HIS:HA   | 42:BH:170:ARG:HD2 | 1.71                     | 0.72              |
| 35:BA:833:U:C5'    | 48:BP:51:PHE:O    | 2.38                     | 0.72              |
| 51:BS:106:ARG:HD2  | 51:BS:108:GLY:N   | 2.04                     | 0.72              |
| 54:BV:19:LYS:HZ1   | 54:BV:20:LEU:HB2  | 1.54                     | 0.72              |
| 1:AA:369:C:O2'     | 1:AA:370:C:H5'    | 1.88                     | 0.71              |
| 1:AA:556:C:H6      | 1:AA:556:C:O5'    | 1.73                     | 0.71              |
| 1:AA:60:A:O2'      | 1:AA:61:G:C5'     | 2.38                     | 0.71              |
| 29:B4:35:VAL:O     | 41:BG:112:PRO:HG2 | 1.88                     | 0.71              |
| 30:B5:52:TYR:O     | 30:B5:53:ALA:CB   | 2.37                     | 0.71              |
| 33:B8:56:GLU:HA    | 33:B8:59:LYS:NZ   | 2.04                     | 0.71              |
| 35:BA:1097:U:H2'   | 35:BA:1098:A:H5'  | 1.70                     | 0.71              |
| 35:BA:1224:C:H6    | 35:BA:1224:C:O5'  | 1.73                     | 0.71              |
| 35:BA:1954:G:N2    | 35:BA:1986:A:OP1  | 2.22                     | 0.71              |
| 35:BA:2310:A:O2'   | 35:BA:2311:A:H5'' | 1.90                     | 0.71              |
| 38:BD:70:TRP:CH2   | 38:BD:150:LYS:HA  | 2.25                     | 0.71              |
| 49:BQ:56:ARG:HG3   | 49:BQ:56:ARG:HH11 | 1.52                     | 0.71              |
| 50:BR:55:ALA:HB2   | 50:BR:79:LEU:HD11 | 1.72                     | 0.71              |
| 35:BA:2873:A:C2    | 50:BR:6:SER:HB2   | 2.25                     | 0.71              |
| 52:BT:95:ARG:HB3   | 52:BT:95:ARG:NH1  | 2.05                     | 0.71              |
| 55:BW:1:MET:HG2    | 55:BW:2:GLU:N     | 2.03                     | 0.71              |
| 1:AA:1152:A:O2'    | 1:AA:1153:C:C5'   | 2.37                     | 0.71              |
| 1:AA:1237:C:O2'    | 1:AA:1335:C:C4'   | 2.38                     | 0.71              |
| 1:AA:123:C:OP1     | 1:AA:311:C:O2'    | 2.07                     | 0.71              |
| 19:AS:32:LYS:HB3   | 19:AS:50:ALA:HB3  | 1.72                     | 0.71              |
| 20:AT:86:ARG:O     | 20:AT:90:GLN:HG2  | 1.90                     | 0.71              |
| 25:B0:78:TYR:O     | 25:B0:79:VAL:HG23 | 1.90                     | 0.71              |
| 35:BA:1405:U:H2'   | 35:BA:1406:U:C6   | 2.25                     | 0.71              |
| 37:BC:51:ASP:HB3   | 37:BC:57:GLN:OE1  | 1.91                     | 0.71              |
| 41:BG:7:LEU:O      | 41:BG:9:ARG:N     | 2.23                     | 0.71              |
| 48:BP:114:ILE:HD12 | 48:BP:114:ILE:C   | 2.10                     | 0.71              |
| 48:BP:16:ARG:CB    | 48:BP:16:ARG:HH11 | 2.03                     | 0.71              |
| 3:AC:119:ARG:O     | 3:AC:122:GLU:HB2  | 1.90                     | 0.71              |
| 3:AC:68:VAL:HG12   | 3:AC:70:VAL:HG13  | 1.72                     | 0.71              |
| 10:AJ:90:LEU:H     | 10:AJ:91:PRO:HD3  | 1.53                     | 0.71              |
| 14:AN:13:THR:N     | 14:AN:14:PRO:HD2  | 2.04                     | 0.71              |
| 24:AY:507:TYR:HE1  | 24:AY:572:TYR:HA  | 1.55                     | 0.71              |
| 35:BA:1646:C:H5'   | 35:BA:1647:G:H5'' | 1.70                     | 0.71              |
| 35:BA:1994:C:H6    | 35:BA:1994:C:O5'  | 1.74                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:652:C:C2    | 35:BA:653:A:H8     | 2.08                     | 0.71              |
| 35:BA:689:A:O2'   | 35:BA:690:G:C5'    | 2.32                     | 0.71              |
| 42:BH:3:ARG:HG2   | 42:BH:4:ILE:O      | 1.90                     | 0.71              |
| 42:BH:70:THR:HG22 | 42:BH:74:ASN:HD21  | 1.55                     | 0.71              |
| 51:BS:15:ARG:HH11 | 51:BS:15:ARG:CB    | 2.01                     | 0.71              |
| 52:BT:29:ARG:N    | 52:BT:45:PHE:O     | 2.23                     | 0.71              |
| 1:AA:1525:G:H2'   | 1:AA:1526:G:H5'    | 1.71                     | 0.71              |
| 1:AA:39:G:O6      | 1:AA:547:A:H2'     | 1.90                     | 0.71              |
| 6:AF:28:ARG:HG3   | 6:AF:28:ARG:HH11   | 1.55                     | 0.71              |
| 10:AJ:9:ARG:HG2   | 10:AJ:69:ASN:OD1   | 1.90                     | 0.71              |
| 25:B0:14:ARG:CG   | 25:B0:14:ARG:HH11  | 2.01                     | 0.71              |
| 28:B3:1:MET:CB    | 28:B3:2:PRO:HD2    | 2.19                     | 0.71              |
| 29:B4:15:ILE:HD13 | 29:B4:33:VAL:CB    | 2.19                     | 0.71              |
| 33:B8:48:PHE:O    | 33:B8:49:VAL:HG22  | 1.90                     | 0.71              |
| 58:BZ:46:LYS:O    | 58:BZ:46:LYS:HD2   | 1.91                     | 0.71              |
| 2:AB:20:GLU:HA    | 2:AB:20:GLU:OE1    | 1.89                     | 0.71              |
| 26:B1:75:GLU:HA   | 26:B1:78:LYS:HD2   | 1.71                     | 0.71              |
| 35:BA:1540:U:H3'  | 35:BA:1541:G:C3'   | 2.14                     | 0.71              |
| 35:BA:1748:G:H5'  | 35:BA:1748:G:H8    | 1.56                     | 0.71              |
| 35:BA:2756:U:H1'  | 35:BA:2757:A:P     | 2.30                     | 0.71              |
| 35:BA:605:C:C2'   | 35:BA:606:U:C5'    | 2.69                     | 0.71              |
| 25:B0:26:TYR:HE2  | 35:BA:857:C:H1'    | 1.54                     | 0.71              |
| 35:BA:859:G:O2'   | 35:BA:916:G:O6     | 2.08                     | 0.71              |
| 41:BG:104:GLU:HB3 | 41:BG:105:LYS:CE   | 2.19                     | 0.71              |
| 48:BP:16:ARG:HD3  | 48:BP:16:ARG:O     | 1.91                     | 0.71              |
| 58:BZ:123:ASP:O   | 58:BZ:124:ILE:HG23 | 1.89                     | 0.71              |
| 1:AA:495:A:H1'    | 1:AA:496:A:N9      | 2.04                     | 0.71              |
| 1:AA:89:C:H1'     | 1:AA:90:U:OP1      | 1.91                     | 0.71              |
| 11:AK:40:ILE:HG23 | 11:AK:75:TYR:CD2   | 2.26                     | 0.71              |
| 1:AA:1305:G:OP1   | 21:AU:2:GLY:CA     | 2.38                     | 0.71              |
| 25:B0:79:VAL:HG12 | 25:B0:79:VAL:O     | 1.90                     | 0.71              |
| 30:B5:52:TYR:O    | 30:B5:53:ALA:HB3   | 1.89                     | 0.71              |
| 35:BA:1210:A:H5'' | 35:BA:1212:G:O4'   | 1.91                     | 0.71              |
| 35:BA:1318:C:H3'  | 35:BA:1319:G:H5''  | 1.73                     | 0.71              |
| 35:BA:1806:C:C2'  | 35:BA:1807:G:H5'   | 2.20                     | 0.71              |
| 35:BA:39:C:C2'    | 35:BA:40:C:H5'     | 2.20                     | 0.71              |
| 35:BA:526:A:O2'   | 35:BA:2043:C:C2'   | 2.38                     | 0.71              |
| 35:BA:688:U:C2'   | 35:BA:689:A:H5'    | 2.20                     | 0.71              |
| 38:BD:43:ARG:HB3  | 38:BD:54:ARG:HB2   | 1.71                     | 0.71              |
| 46:BN:7:LYS:O     | 46:BN:9:VAL:HG23   | 1.89                     | 0.71              |
| 49:BQ:17:LEU:HD21 | 49:BQ:96:VAL:HG13  | 1.71                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:BU:85:LYS:HD3   | 53:BU:117:GLN:HE21 | 1.56                     | 0.71              |
| 58:BZ:149:SER:OG   | 58:BZ:173:ALA:HA   | 1.90                     | 0.71              |
| 1:AA:1149:C:H2'    | 1:AA:1150:U:C6     | 2.25                     | 0.71              |
| 1:AA:1279:A:C4'    | 1:AA:1280:A:OP1    | 2.39                     | 0.71              |
| 1:AA:1305:G:O2'    | 1:AA:1306:A:H8     | 1.69                     | 0.71              |
| 1:AA:973:G:C4      | 10:AJ:55:LYS:HE3   | 2.25                     | 0.71              |
| 1:AA:538:G:H5''    | 12:AL:114:LYS:HB2  | 1.72                     | 0.71              |
| 17:AQ:67:LYS:O     | 17:AQ:68:ARG:HB2   | 1.90                     | 0.71              |
| 27:B2:47:ASN:O     | 27:B2:49:LYS:N     | 2.24                     | 0.71              |
| 29:B4:15:ILE:HD11  | 29:B4:31:ILE:HG23  | 1.71                     | 0.71              |
| 35:BA:2364:C:O2'   | 35:BA:2365:G:H5'   | 1.89                     | 0.71              |
| 41:BG:66:GLN:CD    | 41:BG:94:LEU:HG    | 2.11                     | 0.71              |
| 48:BP:51:PHE:CD2   | 48:BP:53:GLY:HA3   | 2.26                     | 0.71              |
| 33:B8:15:LYS:HB2   | 48:BP:65:ARG:HH12  | 1.55                     | 0.71              |
| 1:AA:185:A:C6      | 1:AA:186:C:N4      | 2.58                     | 0.71              |
| 1:AA:250:A:H4'     | 1:AA:251:G:O5'     | 1.90                     | 0.71              |
| 1:AA:360:A:O2'     | 1:AA:361:G:C5'     | 2.30                     | 0.71              |
| 9:AI:95:LYS:HE3    | 9:AI:96:LEU:CD2    | 2.21                     | 0.71              |
| 28:B3:22:ALA:HB3   | 28:B3:50:VAL:HG11  | 1.72                     | 0.71              |
| 31:B6:30:THR:HG23  | 31:B6:31:PRO:HD2   | 1.73                     | 0.71              |
| 35:BA:1228:G:H21   | 35:BA:1229:G:H1'   | 1.54                     | 0.71              |
| 35:BA:1713:U:O2'   | 35:BA:1714:G:H5'   | 1.91                     | 0.71              |
| 35:BA:1769:G:C6    | 35:BA:1984:G:O6    | 2.43                     | 0.71              |
| 35:BA:404:C:H4'    | 35:BA:405:U:H5'    | 1.71                     | 0.71              |
| 35:BA:459:U:H2'    | 35:BA:460:A:H5'    | 1.72                     | 0.71              |
| 35:BA:654(F):C:H2' | 35:BA:654(G):C:O4' | 1.91                     | 0.71              |
| 38:BD:35:LYS:HD3   | 38:BD:61:LEU:HB3   | 1.73                     | 0.71              |
| 39:BE:87:GLU:O     | 39:BE:87:GLU:OE1   | 2.09                     | 0.71              |
| 40:BF:132:VAL:HG22 | 40:BF:133:ASN:H    | 1.53                     | 0.71              |
| 44:BK:57:UNK:HA    | 44:BK:67:UNK:HA    | 1.73                     | 0.71              |
| 47:BO:87:ILE:CG2   | 47:BO:91:LEU:HA    | 2.20                     | 0.71              |
| 53:BU:90:VAL:HG11  | 54:BV:39:LEU:CG    | 2.21                     | 0.71              |
| 1:AA:1049:U:H1'    | 1:AA:1050:G:OP2    | 1.90                     | 0.71              |
| 1:AA:558:G:H2'     | 1:AA:559:A:C2      | 2.24                     | 0.71              |
| 1:AA:921:U:H2'     | 1:AA:922:G:O4'     | 1.91                     | 0.71              |
| 2:AB:132:LYS:HA    | 2:AB:135:GLN:HG3   | 1.72                     | 0.71              |
| 2:AB:51:LEU:O      | 2:AB:55:PHE:HB2    | 1.91                     | 0.71              |
| 4:AD:13:ARG:HB3    | 4:AD:38:TYR:O      | 1.90                     | 0.71              |
| 25:B0:37:LEU:HD21  | 25:B0:61:ALA:HB2   | 1.73                     | 0.71              |
| 29:B4:1:MET:HB2    | 36:BB:39:A:N6      | 2.05                     | 0.71              |
| 35:BA:1210:A:C8    | 35:BA:1210:A:H5'   | 2.24                     | 0.71              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:BA:1332:G:N2    | 35:BA:1609:A:HO2'   | 1.89                     | 0.71              |
| 35:BA:1639:U:C2'   | 35:BA:1640:C:H5''   | 2.19                     | 0.71              |
| 35:BA:272(H):C:C2' | 35:BA:272(I):U:H5'' | 2.21                     | 0.71              |
| 35:BA:500:G:N2     | 35:BA:502:A:H3'     | 2.06                     | 0.71              |
| 35:BA:630:G:N2     | 35:BA:632:A:H3'     | 2.06                     | 0.71              |
| 35:BA:930:U:H4'    | 35:BA:931:G:O5'     | 1.91                     | 0.71              |
| 37:BC:55:SER:O     | 37:BC:57:GLN:N      | 2.22                     | 0.71              |
| 37:BC:72:GLN:HA    | 37:BC:72:GLN:HE21   | 1.56                     | 0.71              |
| 38:BD:10:THR:OG1   | 38:BD:13:ARG:HB2    | 1.89                     | 0.71              |
| 48:BP:144:GLU:N    | 48:BP:145:PRO:HD3   | 2.06                     | 0.71              |
| 50:BR:7:GLY:HA3    | 50:BR:8:ARG:CZ      | 2.21                     | 0.71              |
| 53:BU:108:GLU:HG3  | 54:BV:44:LYS:HD3    | 1.72                     | 0.71              |
| 49:BQ:60:ARG:CG    | 58:BZ:179:ASP:CG    | 2.58                     | 0.71              |
| 1:AA:1176:A:H2'    | 1:AA:1177:G:H8      | 1.55                     | 0.71              |
| 1:AA:1240:U:OP1    | 7:AG:116:ALA:HB2    | 1.91                     | 0.71              |
| 1:AA:1408:A:H5'    | 1:AA:1408:A:H8      | 1.56                     | 0.71              |
| 1:AA:199:G:O2'     | 1:AA:200:G:C5'      | 2.39                     | 0.71              |
| 1:AA:701:C:C5'     | 1:AA:702:A:OP1      | 2.37                     | 0.71              |
| 16:AP:21:VAL:HG13  | 16:AP:33:ILE:HB     | 1.73                     | 0.71              |
| 24:AY:517:LEU:HD11 | 24:AY:564:LYS:CB    | 2.21                     | 0.71              |
| 35:BA:415:A:N1     | 35:BA:2409:G:C6     | 2.59                     | 0.71              |
| 35:BA:248:G:N7     | 35:BA:250:G:C4      | 2.59                     | 0.71              |
| 37:BC:88:GLU:HG3   | 37:BC:89:GLU:H      | 1.55                     | 0.71              |
| 48:BP:71:VAL:HG13  | 48:BP:72:PRO:HD3    | 1.73                     | 0.71              |
| 58:BZ:112:ARG:HD3  | 58:BZ:112:ARG:C     | 2.11                     | 0.71              |
| 1:AA:1176:A:O2'    | 1:AA:1177:G:H5'     | 1.91                     | 0.70              |
| 1:AA:1498:U:C4'    | 1:AA:1499:A:O5'     | 2.39                     | 0.70              |
| 1:AA:548:G:H2'     | 1:AA:549:C:H5'      | 1.72                     | 0.70              |
| 1:AA:563:A:H61     | 1:AA:884:U:H3       | 1.39                     | 0.70              |
| 2:AB:71:VAL:HG21   | 2:AB:162:ILE:HD11   | 1.72                     | 0.70              |
| 1:AA:406:G:H5''    | 4:AD:5:ILE:HG23     | 1.73                     | 0.70              |
| 15:AO:39:LEU:HD13  | 15:AO:56:LEU:HB2    | 1.71                     | 0.70              |
| 22:AV:73:A:H2'     | 22:AV:74:C:H5'      | 1.73                     | 0.70              |
| 24:AY:342:TYR:CE2  | 24:AY:347:GLY:HA2   | 2.26                     | 0.70              |
| 28:B3:59:VAL:HG12  | 28:B3:60:GLU:N      | 2.05                     | 0.70              |
| 30:B5:56:LYS:HD2   | 30:B5:59:GLU:OE2    | 1.89                     | 0.70              |
| 35:BA:83:G:H22     | 35:BA:102:G:H2'     | 1.56                     | 0.70              |
| 35:BA:2753:A:C2'   | 35:BA:2754:U:H5'    | 2.20                     | 0.70              |
| 35:BA:603:A:C4'    | 35:BA:604:G:O5'     | 2.39                     | 0.70              |
| 35:BA:603:A:C1'    | 35:BA:604:G:OP2     | 2.36                     | 0.70              |
| 37:BC:85:LYS:HD2   | 37:BC:151:GLY:HA3   | 1.72                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BN:39:ARG:HH21  | 46:BN:41:ASP:CB    | 2.04                     | 0.70              |
| 1:AA:1039:C:H2'    | 1:AA:1040:U:C6     | 2.26                     | 0.70              |
| 1:AA:1399:C:C2     | 1:AA:1502:A:N6     | 2.59                     | 0.70              |
| 1:AA:495:A:H1'     | 1:AA:496:A:C8      | 2.26                     | 0.70              |
| 1:AA:874:G:C6      | 1:AA:875:C:N4      | 2.59                     | 0.70              |
| 3:AC:167:TRP:CD1   | 3:AC:168:ALA:O     | 2.44                     | 0.70              |
| 4:AD:30:LYS:C      | 4:AD:32:ALA:H      | 1.94                     | 0.70              |
| 24:AY:530:VAL:HG22 | 24:AY:531:GLY:N    | 2.06                     | 0.70              |
| 30:B5:20:ARG:HG2   | 30:B5:23:HIS:CD2   | 2.26                     | 0.70              |
| 35:BA:1808:U:H2'   | 35:BA:1809:A:H5'   | 1.72                     | 0.70              |
| 35:BA:689:A:H2'    | 35:BA:690:G:C5'    | 2.21                     | 0.70              |
| 41:BG:107:LEU:HD11 | 41:BG:177:GLY:O    | 1.90                     | 0.70              |
| 41:BG:83:ARG:H     | 41:BG:83:ARG:HD2   | 1.56                     | 0.70              |
| 52:BT:32:TYR:O     | 52:BT:33:LYS:CB    | 2.39                     | 0.70              |
| 53:BU:55:ARG:HA    | 53:BU:58:ARG:HD2   | 1.72                     | 0.70              |
| 35:BA:71:A:C2      | 56:BX:31:HIS:HE1   | 2.09                     | 0.70              |
| 1:AA:1370:G:O2'    | 1:AA:1371:G:H5'    | 1.92                     | 0.70              |
| 1:AA:774:G:H2'     | 1:AA:775:G:H8      | 1.56                     | 0.70              |
| 1:AA:939:G:H1      | 1:AA:1344:C:H42    | 1.37                     | 0.70              |
| 4:AD:105:VAL:HG21  | 4:AD:126:ILE:HG12  | 1.72                     | 0.70              |
| 1:AA:1305:G:H5'    | 21:AU:4:GLY:HA3    | 1.73                     | 0.70              |
| 35:BA:1416:G:O2'   | 35:BA:1417:C:C5    | 2.30                     | 0.70              |
| 35:BA:1649:G:C2'   | 35:BA:1650:G:H5'   | 2.20                     | 0.70              |
| 35:BA:796:C:H2'    | 35:BA:797:C:C6     | 2.26                     | 0.70              |
| 35:BA:8:A:H2'      | 35:BA:9:U:C5       | 2.26                     | 0.70              |
| 40:BF:6:VAL:CG1    | 40:BF:7:TYR:H      | 1.98                     | 0.70              |
| 57:BY:28:LYS:CD    | 57:BY:28:LYS:N     | 2.49                     | 0.70              |
| 58:BZ:152:ALA:HB2  | 58:BZ:169:GLU:O    | 1.91                     | 0.70              |
| 1:AA:1001(A):G:H2' | 1:AA:1002:G:O4'    | 1.90                     | 0.70              |
| 4:AD:129:ASN:ND2   | 4:AD:145:GLU:H     | 1.88                     | 0.70              |
| 9:AI:13:ALA:HA     | 9:AI:67:GLY:O      | 1.91                     | 0.70              |
| 24:AY:122:TRP:CD2  | 24:AY:157:LEU:HD12 | 2.26                     | 0.70              |
| 26:B1:52:ARG:O     | 26:B1:53:VAL:HG22  | 1.92                     | 0.70              |
| 35:BA:1778:U:H2'   | 35:BA:1784:A:N6    | 2.07                     | 0.70              |
| 35:BA:1808:U:O5'   | 35:BA:1808:U:H6    | 1.74                     | 0.70              |
| 35:BA:2007:C:H2'   | 35:BA:2008:C:H6    | 1.56                     | 0.70              |
| 35:BA:27:G:H22     | 35:BA:512:G:C2'    | 1.97                     | 0.70              |
| 35:BA:689:A:C2'    | 35:BA:690:G:C5'    | 2.63                     | 0.70              |
| 35:BA:774:A:H2     | 35:BA:787:U:HO2'   | 1.36                     | 0.70              |
| 35:BA:893:C:H2'    | 35:BA:894:C:H6     | 1.56                     | 0.70              |
| 42:BH:9:ILE:HG22   | 42:BH:10:PRO:CA    | 2.20                     | 0.70              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:BP:34:GLY:O     | 48:BP:35:HIS:HB2  | 1.91                     | 0.70              |
| 54:BV:19:LYS:NZ    | 54:BV:20:LEU:H    | 1.89                     | 0.70              |
| 1:AA:489:C:H2'     | 1:AA:490:G:C8     | 2.26                     | 0.70              |
| 1:AA:543:C:O2'     | 1:AA:544:G:C5'    | 2.39                     | 0.70              |
| 1:AA:1103:C:OP1    | 2:AB:96:ARG:NH2   | 2.23                     | 0.70              |
| 3:AC:118:GLN:O     | 3:AC:121:ALA:N    | 2.25                     | 0.70              |
| 10:AJ:50:ILE:HA    | 10:AJ:60:ARG:HG2  | 1.73                     | 0.70              |
| 15:AO:17:ARG:HD3   | 15:AO:26:GLU:HG3  | 1.71                     | 0.70              |
| 15:AO:82:ILE:CD1   | 15:AO:88:ARG:HB2  | 2.19                     | 0.70              |
| 26:B1:75:GLU:O     | 26:B1:78:LYS:CD   | 2.39                     | 0.70              |
| 35:BA:1884:A:C2'   | 35:BA:1885:A:H5'' | 2.21                     | 0.70              |
| 35:BA:2715:C:HO2'  | 35:BA:2716:U:H5'  | 1.56                     | 0.70              |
| 35:BA:603:A:C8     | 35:BA:655:A:N6    | 2.59                     | 0.70              |
| 35:BA:743:G:H2'    | 35:BA:744:G:O5'   | 1.90                     | 0.70              |
| 35:BA:968:G:O2'    | 35:BA:969:U:C5'   | 2.30                     | 0.70              |
| 37:BC:15:VAL:O     | 37:BC:16:ASP:HB3  | 1.92                     | 0.70              |
| 52:BT:29:ARG:HH11  | 52:BT:88:ILE:HD11 | 1.53                     | 0.70              |
| 1:AA:109:A:C6      | 1:AA:326:G:C6     | 2.78                     | 0.70              |
| 1:AA:1279:A:H4'    | 1:AA:1280:A:OP1   | 1.92                     | 0.70              |
| 1:AA:946:A:O2'     | 1:AA:947:G:H5'    | 1.92                     | 0.70              |
| 2:AB:212:GLN:HG2   | 2:AB:235:SER:HB2  | 1.73                     | 0.70              |
| 24:AY:25:LYS:NZ    | 24:AY:86:GLY:N    | 2.40                     | 0.70              |
| 31:B6:7:ILE:CG2    | 31:B6:27:LYS:HZ3  | 1.93                     | 0.70              |
| 35:BA:144:C:H2'    | 35:BA:145:G:H8    | 1.56                     | 0.70              |
| 35:BA:1963:U:C2'   | 35:BA:1963:U:O2   | 2.39                     | 0.70              |
| 35:BA:2362:G:C2'   | 35:BA:2363:C:H5'  | 2.21                     | 0.70              |
| 35:BA:599:G:H2'    | 35:BA:600:G:H5'   | 1.71                     | 0.70              |
| 42:BH:149:ARG:HD3  | 42:BH:164:TYR:HE1 | 1.56                     | 0.70              |
| 48:BP:115:LEU:HD23 | 48:BP:116:GLY:N   | 2.07                     | 0.70              |
| 9:AI:65:VAL:HG21   | 9:AI:73:GLN:CB    | 2.13                     | 0.70              |
| 15:AO:87:ILE:CG2   | 15:AO:88:ARG:H    | 2.03                     | 0.70              |
| 24:AY:461:ILE:O    | 24:AY:465:ARG:HB2 | 1.92                     | 0.70              |
| 24:AY:14:ASN:ND2   | 24:AY:80:ASN:HD22 | 1.89                     | 0.70              |
| 25:B0:19:LYS:NZ    | 25:B0:41:ARG:NH2  | 2.39                     | 0.70              |
| 25:B0:53:MET:SD    | 25:B0:57:PHE:HA   | 2.31                     | 0.70              |
| 34:B9:10:ILE:O     | 34:B9:11:CYS:HB3  | 1.91                     | 0.70              |
| 34:B9:1:MET:SD     | 34:B9:31:LYS:HB3  | 2.31                     | 0.70              |
| 35:BA:880:G:C2'    | 35:BA:881:G:H5''  | 2.21                     | 0.70              |
| 40:BF:101:LEU:HD12 | 40:BF:102:PRO:HD2 | 1.74                     | 0.70              |
| 41:BG:61:ALA:CB    | 41:BG:68:PRO:HD3  | 2.20                     | 0.70              |
| 51:BS:106:ARG:HB3  | 51:BS:106:ARG:NH1 | 2.02                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:BS:28:VAL:HG12  | 51:BS:29:PHE:N     | 2.06                     | 0.70              |
| 1:AA:1047:G:O2'    | 1:AA:1048:G:H5'    | 1.91                     | 0.70              |
| 1:AA:1075:C:C2'    | 1:AA:1076:C:H5'    | 2.22                     | 0.70              |
| 1:AA:1368:G:O2'    | 1:AA:1369:C:H5'    | 1.92                     | 0.70              |
| 1:AA:940:C:H2'     | 1:AA:941:G:H5'     | 1.73                     | 0.70              |
| 2:AB:36:ARG:O      | 2:AB:37:ASN:CB     | 2.40                     | 0.70              |
| 2:AB:82:ARG:HA     | 2:AB:92:TYR:CE1    | 2.26                     | 0.70              |
| 3:AC:187:ALA:HB2   | 3:AC:198:VAL:HB    | 1.74                     | 0.70              |
| 22:AV:40:C:H2'     | 22:AV:41:C:C6      | 2.26                     | 0.70              |
| 24:AY:86:GLY:O     | 24:AY:117:GLN:HG2  | 1.92                     | 0.70              |
| 24:AY:8:ASP:HB3    | 24:AY:11:ARG:HD2   | 1.74                     | 0.70              |
| 26:B1:57:GLU:C     | 26:B1:58:ILE:HG13  | 2.12                     | 0.70              |
| 35:BA:1786:A:H1'   | 35:BA:1938:A:H62   | 1.54                     | 0.70              |
| 35:BA:1941:C:C2'   | 35:BA:1942:C:H5'   | 2.22                     | 0.70              |
| 35:BA:658:C:H2'    | 35:BA:659:C:C6     | 2.27                     | 0.70              |
| 35:BA:968:G:H2'    | 35:BA:969:U:C6     | 2.27                     | 0.70              |
| 58:BZ:19:ARG:NH1   | 58:BZ:84:GLU:O     | 2.25                     | 0.70              |
| 1:AA:46:G:O2'      | 1:AA:365:U:C1'     | 2.40                     | 0.70              |
| 7:AG:36:LYS:HG2    | 7:AG:37:ASN:N      | 2.04                     | 0.70              |
| 24:AY:111:SER:OG   | 24:AY:141:LYS:HD2  | 1.92                     | 0.70              |
| 24:AY:15:ILE:O     | 24:AY:81:ILE:HA    | 1.92                     | 0.70              |
| 24:AY:301:ILE:HG22 | 24:AY:332:SER:HB2  | 1.73                     | 0.70              |
| 35:BA:1058:G:H2'   | 35:BA:1059:G:C5'   | 2.22                     | 0.70              |
| 35:BA:171:G:O2'    | 35:BA:172:C:H5'    | 1.91                     | 0.70              |
| 35:BA:2870:C:H2'   | 35:BA:2871:C:O4'   | 1.92                     | 0.70              |
| 37:BC:153:ILE:HG23 | 37:BC:161:ARG:NH1  | 2.06                     | 0.70              |
| 39:BE:34:VAL:HG22  | 39:BE:48:GLN:HE21  | 1.56                     | 0.70              |
| 33:B8:15:LYS:HD2   | 48:BP:65:ARG:HH22  | 1.56                     | 0.70              |
| 58:BZ:104:PHE:HB3  | 58:BZ:141:VAL:HG21 | 1.73                     | 0.70              |
| 1:AA:110:C:C2'     | 1:AA:111:G:H5'     | 2.22                     | 0.70              |
| 4:AD:189:PRO:HB2   | 4:AD:194:LEU:HD21  | 1.73                     | 0.70              |
| 11:AK:82:VAL:HG13  | 11:AK:108:ILE:HA   | 1.74                     | 0.70              |
| 12:AL:123:LYS:H    | 12:AL:123:LYS:HE3  | 1.56                     | 0.70              |
| 24:AY:149:VAL:O    | 24:AY:153:MET:HG3  | 1.92                     | 0.70              |
| 35:BA:110:G:C2'    | 35:BA:111:A:H5'    | 2.22                     | 0.70              |
| 35:BA:2176:A:C4'   | 35:BA:2177:C:OP1   | 2.37                     | 0.70              |
| 35:BA:461:C:C2'    | 35:BA:462:C:C5'    | 2.69                     | 0.70              |
| 41:BG:104:GLU:OE2  | 41:BG:107:LEU:HD12 | 1.92                     | 0.70              |
| 30:B5:44:THR:HG21  | 50:BR:101:ALA:HB2  | 1.74                     | 0.70              |
| 52:BT:50:ILE:HA    | 52:BT:99:LEU:CD1   | 2.22                     | 0.70              |
| 55:BW:71:VAL:O     | 55:BW:71:VAL:HG23  | 1.90                     | 0.70              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 57:BY:11:ASP:O      | 57:BY:28:LYS:HE3   | 1.92                     | 0.70              |
| 1:AA:57:G:H2'       | 1:AA:58:C:H6       | 1.52                     | 0.69              |
| 2:AB:156:LYS:O      | 2:AB:157:ARG:HB2   | 1.91                     | 0.69              |
| 2:AB:96:ARG:O       | 2:AB:96:ARG:HG3    | 1.92                     | 0.69              |
| 7:AG:26:PHE:CE2     | 7:AG:30:ILE:HD11   | 2.26                     | 0.69              |
| 19:AS:63:THR:HG23   | 19:AS:64:GLU:N     | 2.06                     | 0.69              |
| 24:AY:386:GLY:CA    | 24:AY:402:ILE:HG12 | 2.21                     | 0.69              |
| 25:B0:10:THR:O      | 25:B0:11:ARG:HG3   | 1.92                     | 0.69              |
| 25:B0:27:GLU:CD     | 25:B0:27:GLU:N     | 2.45                     | 0.69              |
| 25:B0:19:LYS:HZ3    | 25:B0:41:ARG:NH2   | 1.90                     | 0.69              |
| 27:B2:16:LEU:HD23   | 27:B2:20:GLU:HG2   | 1.71                     | 0.69              |
| 28:B3:35:ARG:HD3    | 28:B3:37:LEU:HD21  | 1.73                     | 0.69              |
| 29:B4:14:ILE:HG22   | 29:B4:14:ILE:O     | 1.92                     | 0.69              |
| 31:B6:41:PRO:HD2    | 31:B6:45:LYS:HA    | 1.74                     | 0.69              |
| 35:BA:1696:G:C2'    | 35:BA:1697:G:H5'   | 2.22                     | 0.69              |
| 35:BA:630:G:C4      | 35:BA:632:A:OP2    | 2.45                     | 0.69              |
| 35:BA:702:G:H2'     | 35:BA:703:U:H5'    | 1.74                     | 0.69              |
| 35:BA:89:G:H3'      | 35:BA:90:U:C5'     | 2.21                     | 0.69              |
| 49:BQ:54:MET:HB3    | 49:BQ:64:ILE:HD13  | 1.72                     | 0.69              |
| 1:AA:1442(A):G:C6   | 52:BT:118:ARG:HB2  | 2.26                     | 0.69              |
| 47:BO:77:ILE:HD13   | 52:BT:74:ARG:HD3   | 1.74                     | 0.69              |
| 1:AA:264:U:C2'      | 1:AA:265:G:C5'     | 2.65                     | 0.69              |
| 24:AY:84:THR:HG23   | 24:AY:85:PRO:CD    | 2.22                     | 0.69              |
| 27:B2:70:GLN:NE2    | 27:B2:71:ASN:H     | 1.90                     | 0.69              |
| 29:B4:31:ILE:HG12   | 29:B4:32:TYR:N     | 2.07                     | 0.69              |
| 34:B9:10:ILE:HD13   | 34:B9:34:GLN:HE22  | 1.56                     | 0.69              |
| 35:BA:1221(A):C:O2' | 35:BA:1222:C:H5'   | 1.93                     | 0.69              |
| 35:BA:1289:C:O2'    | 35:BA:1290:C:H5'   | 1.92                     | 0.69              |
| 35:BA:1300:U:C4'    | 35:BA:1301:A:O5'   | 2.34                     | 0.69              |
| 35:BA:1516:C:H2'    | 35:BA:1517:G:H5'   | 1.73                     | 0.69              |
| 35:BA:2836:U:H2'    | 35:BA:2837:G:C8    | 2.27                     | 0.69              |
| 37:BC:183:PRO:HG2   | 37:BC:184:GLU:OE2  | 1.92                     | 0.69              |
| 35:BA:2580:U:H5'    | 39:BE:131:ALA:CB   | 2.23                     | 0.69              |
| 42:BH:168:PRO:CA    | 42:BH:170:ARG:NH2  | 2.54                     | 0.69              |
| 1:AA:100:C:H2'      | 1:AA:101:A:C8      | 2.27                     | 0.69              |
| 24:AY:551:GLN:O     | 24:AY:559:PRO:HA   | 1.93                     | 0.69              |
| 29:B4:43:TYR:C      | 29:B4:45:GLY:H     | 1.96                     | 0.69              |
| 35:BA:1539:G:C5     | 35:BA:1540:U:H1'   | 2.27                     | 0.69              |
| 35:BA:1998:G:H2'    | 35:BA:1999:C:C6    | 2.27                     | 0.69              |
| 37:BC:100:ILE:C     | 37:BC:102:GLN:H    | 1.96                     | 0.69              |
| 37:BC:80:LYS:HE3    | 37:BC:120:VAL:CG1  | 2.14                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BG:136:ARG:O   | 41:BG:136:ARG:HG3 | 1.92                     | 0.69              |
| 58:BZ:185:GLU:C   | 58:BZ:187:ALA:N   | 2.44                     | 0.69              |
| 58:BZ:17:ALA:HA   | 58:BZ:20:ARG:HG2  | 1.74                     | 0.69              |
| 1:AA:542:G:H2'    | 1:AA:543:C:C6     | 2.28                     | 0.69              |
| 1:AA:982:U:H4'    | 1:AA:983:A:O5'    | 1.92                     | 0.69              |
| 25:B0:53:MET:CG   | 25:B0:57:PHE:HA   | 2.23                     | 0.69              |
| 29:B4:56:VAL:HG13 | 29:B4:57:GLU:HG3  | 1.75                     | 0.69              |
| 35:BA:1104:C:O2'  | 35:BA:1105:U:H5'  | 1.92                     | 0.69              |
| 25:B0:43:THR:H    | 35:BA:2331:G:H4'  | 1.57                     | 0.69              |
| 35:BA:2645:G:C3'  | 35:BA:2646:C:H5'  | 2.20                     | 0.69              |
| 56:BX:35:THR:HG22 | 56:BX:37:THR:N    | 2.07                     | 0.69              |
| 1:AA:1027:C:H2'   | 1:AA:1028:C:O4'   | 1.92                     | 0.69              |
| 12:AL:6:THR:OG1   | 12:AL:9:GLN:HG3   | 1.92                     | 0.69              |
| 29:B4:15:ILE:CD1  | 29:B4:33:VAL:HB   | 2.18                     | 0.69              |
| 35:BA:1290:C:O2'  | 35:BA:1291:C:H5'  | 1.93                     | 0.69              |
| 47:BO:2:ILE:HB    | 47:BO:33:ALA:HB3  | 1.75                     | 0.69              |
| 51:BS:13:ARG:CG   | 51:BS:14:VAL:H    | 2.04                     | 0.69              |
| 35:BA:2875:C:O2'  | 52:BT:5:ALA:HB3   | 1.92                     | 0.69              |
| 1:AA:1072:G:H2'   | 1:AA:1073:U:C6    | 2.26                     | 0.69              |
| 1:AA:1139:G:H5'   | 1:AA:1140:C:OP1   | 1.92                     | 0.69              |
| 1:AA:360:A:HO2'   | 1:AA:361:G:H5'    | 1.58                     | 0.69              |
| 1:AA:60:A:C4'     | 1:AA:61:G:O5'     | 2.40                     | 0.69              |
| 7:AG:50:ILE:HG23  | 7:AG:58:PRO:HG3   | 1.74                     | 0.69              |
| 25:B0:43:THR:O    | 25:B0:43:THR:CG2  | 2.40                     | 0.69              |
| 26:B1:82:LEU:O    | 26:B1:83:GLU:CB   | 2.40                     | 0.69              |
| 27:B2:2:LYS:HD2   | 27:B2:5:GLU:HG3   | 1.74                     | 0.69              |
| 35:BA:176:G:C2'   | 35:BA:177:G:C5'   | 2.65                     | 0.69              |
| 26:B1:45:ASN:ND2  | 35:BA:2090:G:H21  | 1.89                     | 0.69              |
| 35:BA:806:C:OP2   | 48:BP:39:LYS:HG3  | 1.91                     | 0.69              |
| 42:BH:3:ARG:CB    | 42:BH:3:ARG:NH1   | 2.41                     | 0.69              |
| 1:AA:1306:A:N6    | 1:AA:1331:G:H1'   | 2.07                     | 0.69              |
| 1:AA:1337:G:H5''  | 1:AA:1338:G:OP1   | 1.93                     | 0.69              |
| 1:AA:688:G:C2'    | 1:AA:689:C:H5'    | 2.22                     | 0.69              |
| 1:AA:942:G:H2'    | 1:AA:943:U:C6     | 2.28                     | 0.69              |
| 2:AB:16:HIS:CE1   | 2:AB:210:SER:CA   | 2.76                     | 0.69              |
| 6:AF:97:PHE:HD2   | 18:AR:31:LEU:HD21 | 1.57                     | 0.69              |
| 1:AA:973:G:H1'    | 10:AJ:55:LYS:NZ   | 2.07                     | 0.69              |
| 24:AY:138:LYS:HG2 | 61:AY:701:GCP:C5  | 2.22                     | 0.69              |
| 25:B0:10:THR:C    | 25:B0:11:ARG:HG3  | 2.13                     | 0.69              |
| 27:B2:16:LEU:CD2  | 27:B2:20:GLU:CG   | 2.45                     | 0.69              |
| 35:BA:1301:A:H2'  | 35:BA:1302:A:H3'  | 1.75                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BC:80:LYS:HG3  | 37:BC:120:VAL:CG1  | 2.22                     | 0.69              |
| 57:BY:84:ARG:NH2  | 57:BY:97:ARG:HB3   | 2.07                     | 0.69              |
| 58:BZ:152:ALA:O   | 58:BZ:155:LEU:HD22 | 1.93                     | 0.69              |
| 1:AA:688:G:O2'    | 1:AA:689:C:C5'     | 2.31                     | 0.69              |
| 1:AA:961:U:H5'    | 1:AA:984:C:H1'     | 1.75                     | 0.69              |
| 2:AB:33:TYR:HB3   | 2:AB:41:ILE:HG22   | 1.75                     | 0.69              |
| 3:AC:130:VAL:HG13 | 3:AC:157:ILE:HG22  | 1.74                     | 0.69              |
| 3:AC:15:THR:CG2   | 3:AC:181:ASN:HA    | 2.23                     | 0.69              |
| 1:AA:921:U:O2'    | 5:AE:19:MET:O      | 2.11                     | 0.69              |
| 11:AK:56:GLY:O    | 11:AK:89:ALA:HB1   | 1.92                     | 0.69              |
| 24:AY:98:MET:HG2  | 24:AY:125:ALA:HA   | 1.74                     | 0.69              |
| 35:BA:1222:C:O2'  | 35:BA:1223:G:C5'   | 2.35                     | 0.69              |
| 35:BA:2201:C:H2'  | 35:BA:2202:C:H6    | 1.57                     | 0.69              |
| 35:BA:259:G:HO2'  | 35:BA:260:G:H5'    | 1.55                     | 0.69              |
| 35:BA:652:C:C2    | 35:BA:653:A:C8     | 2.81                     | 0.69              |
| 37:BC:122:GLY:O   | 37:BC:127:LYS:CE   | 2.41                     | 0.69              |
| 41:BG:7:LEU:HD13  | 41:BG:100:TRP:CE3  | 2.27                     | 0.69              |
| 48:BP:115:LEU:CG  | 48:BP:116:GLY:H    | 2.05                     | 0.69              |
| 52:BT:32:TYR:CD2  | 52:BT:81:PRO:O     | 1.95                     | 0.69              |
| 1:AA:114:U:O5'    | 1:AA:114:U:H6      | 1.75                     | 0.69              |
| 1:AA:1157:A:C4'   | 1:AA:1158:C:O5'    | 2.40                     | 0.69              |
| 1:AA:199:G:H2'    | 1:AA:200:G:C8      | 2.28                     | 0.69              |
| 1:AA:505:G:H2'    | 1:AA:506:G:C8      | 2.28                     | 0.69              |
| 26:B1:29:GLY:C    | 26:B1:30:VAL:CG2   | 2.62                     | 0.69              |
| 29:B4:66:SER:O    | 29:B4:67:TYR:HB2   | 1.93                     | 0.69              |
| 29:B4:7:PRO:HD3   | 41:BG:66:GLN:HA    | 1.74                     | 0.69              |
| 35:BA:1301:A:O2'  | 35:BA:1302:A:C2'   | 2.30                     | 0.69              |
| 35:BA:1423:G:HO2' | 35:BA:1424:G:H5'   | 1.55                     | 0.69              |
| 38:BD:210:GLY:O   | 38:BD:211:ARG:HB3  | 1.92                     | 0.69              |
| 47:BO:4:PRO:O     | 47:BO:5:GLN:CB     | 2.40                     | 0.69              |
| 1:AA:170:U:O2'    | 1:AA:171:A:H5'     | 1.91                     | 0.69              |
| 3:AC:83:ARG:CG    | 3:AC:84:ILE:H      | 2.05                     | 0.69              |
| 9:AI:25:LYS:O     | 9:AI:26:VAL:HG12   | 1.93                     | 0.69              |
| 9:AI:70:LYS:O     | 9:AI:74:ILE:HG13   | 1.92                     | 0.69              |
| 13:AM:81:LEU:O    | 13:AM:86:CYS:HB3   | 1.92                     | 0.69              |
| 19:AS:88:LYS:O    | 19:AS:90:THR:HG22  | 1.92                     | 0.69              |
| 31:B6:15:GLU:OE2  | 31:B6:41:PRO:HB3   | 1.92                     | 0.69              |
| 31:B6:25:LYS:HZ1  | 33:B8:34:TRP:HZ2   | 1.40                     | 0.69              |
| 35:BA:1041:G:N2   | 35:BA:1114:G:H22   | 1.91                     | 0.69              |
| 35:BA:1446:C:N4   | 35:BA:1465:G:N1    | 2.39                     | 0.69              |
| 35:BA:285:C:H2'   | 35:BA:286:C:C6     | 2.28                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:465:G:H2'    | 35:BA:466:A:C8     | 2.28                     | 0.69              |
| 35:BA:860:U:C2'    | 35:BA:861:A:H5'    | 2.22                     | 0.69              |
| 48:BP:30:THR:HG22  | 48:BP:31:ALA:N     | 2.08                     | 0.69              |
| 50:BR:103:ARG:HH12 | 50:BR:110:PRO:HD3  | 1.58                     | 0.69              |
| 1:AA:539:A:H2'     | 1:AA:540:G:C8      | 2.28                     | 0.69              |
| 1:AA:698:G:H2'     | 1:AA:699:C:C6      | 2.27                     | 0.69              |
| 29:B4:24:THR:O     | 29:B4:25:TYR:CG    | 2.46                     | 0.69              |
| 35:BA:2291:U:H2'   | 35:BA:2292:C:C6    | 2.28                     | 0.69              |
| 35:BA:259:G:C2'    | 35:BA:260:G:H5'    | 2.22                     | 0.69              |
| 35:BA:326:G:HO2'   | 35:BA:327:G:H5'    | 1.57                     | 0.69              |
| 38:BD:76:PRO:HG2   | 38:BD:98:VAL:HG21  | 1.75                     | 0.69              |
| 44:BK:100:UNK:HA   | 44:BK:137:UNK:O    | 1.93                     | 0.69              |
| 48:BP:115:LEU:HG   | 48:BP:116:GLY:H    | 1.58                     | 0.69              |
| 35:BA:907:U:OP1    | 49:BQ:24:GLY:N     | 2.26                     | 0.69              |
| 49:BQ:76:LYS:HB3   | 49:BQ:91:GLU:CG    | 2.23                     | 0.69              |
| 51:BS:66:ALA:HB1   | 51:BS:99:LYS:HG2   | 1.74                     | 0.69              |
| 52:BT:30:VAL:HG12  | 52:BT:31:SER:HB2   | 1.73                     | 0.69              |
| 58:BZ:165:VAL:CG1  | 58:BZ:166:SER:H    | 2.06                     | 0.69              |
| 1:AA:593:G:C2'     | 1:AA:594:G:C5'     | 2.71                     | 0.68              |
| 1:AA:593:G:H2'     | 1:AA:594:G:H5'     | 1.75                     | 0.68              |
| 29:B4:14:ILE:C     | 29:B4:15:ILE:HD12  | 2.12                     | 0.68              |
| 35:BA:34:C:O5'     | 35:BA:34:C:H6      | 1.76                     | 0.68              |
| 29:B4:22:ILE:CG2   | 41:BG:105:LYS:HD3  | 2.23                     | 0.68              |
| 42:BH:30:LYS:HG2   | 42:BH:79:VAL:O     | 1.93                     | 0.68              |
| 49:BQ:54:MET:HB3   | 49:BQ:64:ILE:CD1   | 2.23                     | 0.68              |
| 50:BR:2:ARG:C      | 50:BR:2:ARG:HD2    | 2.13                     | 0.68              |
| 51:BS:23:ARG:HB3   | 51:BS:24:LEU:HD22  | 1.74                     | 0.68              |
| 52:BT:29:ARG:O     | 52:BT:30:VAL:CG2   | 2.37                     | 0.68              |
| 58:BZ:79:ARG:C     | 58:BZ:81:ARG:H     | 1.96                     | 0.68              |
| 1:AA:353:A:C8      | 1:AA:353:A:H5'     | 2.23                     | 0.68              |
| 11:AK:82:VAL:HG11  | 11:AK:108:ILE:HG12 | 1.75                     | 0.68              |
| 13:AM:65:LYS:HD3   | 13:AM:69:GLU:HG3   | 1.75                     | 0.68              |
| 24:AY:53:ASP:HB3   | 24:AY:58:GLU:OE1   | 1.92                     | 0.68              |
| 25:B0:64:ASP:O     | 25:B0:84:LEU:HG    | 1.94                     | 0.68              |
| 35:BA:1383:C:O5'   | 35:BA:1383:C:H6    | 1.75                     | 0.68              |
| 35:BA:1864:U:C2'   | 35:BA:1865:G:H5''  | 2.23                     | 0.68              |
| 35:BA:2524:G:H5'   | 35:BA:2524:G:H8    | 1.57                     | 0.68              |
| 35:BA:262:A:H2'    | 35:BA:263:C:H5'    | 1.75                     | 0.68              |
| 35:BA:45:C:O2      | 35:BA:179:G:N2     | 2.26                     | 0.68              |
| 37:BC:25:GLU:HA    | 37:BC:28:ARG:HD2   | 1.74                     | 0.68              |
| 52:BT:102:ILE:HB   | 52:BT:110:ILE:CD1  | 2.22                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:166:G:H2'     | 1:AA:167:G:H8      | 1.56                     | 0.68              |
| 1:AA:267:C:P       | 17:AQ:67:LYS:HB2   | 2.33                     | 0.68              |
| 1:AA:311:C:HO2'    | 1:AA:312:C:C5'     | 2.07                     | 0.68              |
| 2:AB:145:LEU:HD23  | 2:AB:149:LEU:CD2   | 2.22                     | 0.68              |
| 7:AG:120:ILE:O     | 7:AG:121:ALA:HB3   | 1.94                     | 0.68              |
| 7:AG:49:ILE:HD13   | 7:AG:118:VAL:HA    | 1.76                     | 0.68              |
| 13:AM:118:ALA:HB1  | 19:AS:88:LYS:HZ3   | 1.58                     | 0.68              |
| 24:AY:153:MET:HA   | 24:AY:157:LEU:HD21 | 1.76                     | 0.68              |
| 24:AY:246:ILE:HG23 | 24:AY:255:ILE:HD11 | 1.75                     | 0.68              |
| 35:BA:1296:G:O2'   | 35:BA:1297:C:H5'   | 1.93                     | 0.68              |
| 35:BA:1941:C:H2'   | 35:BA:1942:C:H5'   | 1.75                     | 0.68              |
| 35:BA:1989:G:O2'   | 35:BA:1990:C:H5'   | 1.93                     | 0.68              |
| 35:BA:2409:G:H2'   | 35:BA:2410:G:H8    | 1.57                     | 0.68              |
| 35:BA:326:G:C2'    | 35:BA:327:G:H5'    | 2.22                     | 0.68              |
| 49:BQ:21:THR:HG22  | 49:BQ:23:GLY:O     | 1.93                     | 0.68              |
| 58:BZ:81:ARG:O     | 58:BZ:81:ARG:HG3   | 1.92                     | 0.68              |
| 1:AA:112:G:C2'     | 1:AA:113:G:C5'     | 2.67                     | 0.68              |
| 1:AA:1281:U:C5'    | 1:AA:1282:C:H5     | 1.98                     | 0.68              |
| 4:AD:3:ARG:H       | 4:AD:3:ARG:HD3     | 1.57                     | 0.68              |
| 31:B6:11:LEU:HD13  | 31:B6:11:LEU:N     | 2.09                     | 0.68              |
| 31:B6:53:LYS:CD    | 31:B6:54:ILE:H     | 2.05                     | 0.68              |
| 35:BA:1062:G:H1    | 35:BA:1075:C:N4    | 1.91                     | 0.68              |
| 35:BA:1054:A:C6    | 35:BA:1106:G:O6    | 2.46                     | 0.68              |
| 35:BA:1223:G:C6    | 35:BA:1227:G:O6    | 2.47                     | 0.68              |
| 35:BA:141:A:H8     | 35:BA:1408:C:O2'   | 1.73                     | 0.68              |
| 35:BA:248:G:N7     | 35:BA:250:G:N3     | 2.41                     | 0.68              |
| 39:BE:65:GLY:HA2   | 39:BE:70:ALA:HB2   | 1.76                     | 0.68              |
| 40:BF:123:LEU:HD12 | 40:BF:124:LEU:H    | 1.58                     | 0.68              |
| 48:BP:38:GLN:O     | 48:BP:39:LYS:HB2   | 1.91                     | 0.68              |
| 50:BR:4:LEU:O      | 50:BR:4:LEU:CG     | 2.41                     | 0.68              |
| 50:BR:59:ASP:O     | 50:BR:60:LEU:HB3   | 1.94                     | 0.68              |
| 51:BS:104:GLY:O    | 51:BS:106:ARG:N    | 2.27                     | 0.68              |
| 52:BT:3:ARG:O      | 52:BT:7:ILE:HG13   | 1.93                     | 0.68              |
| 7:AG:47:CYS:HA     | 7:AG:50:ILE:HG22   | 1.76                     | 0.68              |
| 12:AL:75:HIS:HD2   | 12:AL:77:LEU:H     | 1.40                     | 0.68              |
| 13:AM:101:GLN:HE21 | 13:AM:101:GLN:N    | 1.90                     | 0.68              |
| 24:AY:238:THR:HG22 | 24:AY:241:GLU:CG   | 2.24                     | 0.68              |
| 25:B0:66:VAL:CG1   | 25:B0:67:VAL:N     | 2.57                     | 0.68              |
| 29:B4:33:VAL:O     | 29:B4:34:GLU:CB    | 2.40                     | 0.68              |
| 35:BA:15:G:O2'     | 35:BA:16:G:C5'     | 2.36                     | 0.68              |
| 26:B1:25:LYS:HD3   | 35:BA:2396:G:O5'   | 1.94                     | 0.68              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:327:G:HO2'   | 35:BA:328:U:H5'   | 1.58                     | 0.68              |
| 35:BA:699:A:O2'    | 35:BA:700:G:H5'   | 1.94                     | 0.68              |
| 35:BA:896:A:C1'    | 58:BZ:176:PRO:CG  | 2.69                     | 0.68              |
| 40:BF:3:GLU:CA     | 40:BF:24:LEU:HG   | 2.24                     | 0.68              |
| 57:BY:76:CYS:HG    | 57:BY:77:PRO:HD2  | 1.58                     | 0.68              |
| 58:BZ:63:ASP:HB2   | 58:BZ:65:GLN:HE21 | 1.59                     | 0.68              |
| 2:AB:168:THR:HG21  | 2:AB:191:ASP:O    | 1.93                     | 0.68              |
| 7:AG:125:MET:O     | 7:AG:128:ALA:HB3  | 1.93                     | 0.68              |
| 15:AO:17:ARG:HH11  | 15:AO:17:ARG:HG3  | 1.58                     | 0.68              |
| 35:BA:1642:G:O2'   | 35:BA:1643:G:H5'  | 1.94                     | 0.68              |
| 35:BA:2009:G:C2    | 35:BA:2010:G:C8   | 2.82                     | 0.68              |
| 38:BD:166:GLN:HE21 | 38:BD:166:GLN:N   | 1.92                     | 0.68              |
| 38:BD:65:ILE:HD11  | 38:BD:67:PHE:CD2  | 2.28                     | 0.68              |
| 39:BE:34:VAL:CG2   | 39:BE:48:GLN:HE21 | 2.06                     | 0.68              |
| 41:BG:6:ALA:HB1    | 41:BG:105:LYS:HZ2 | 1.58                     | 0.68              |
| 48:BP:85:LEU:HD22  | 48:BP:117:GLU:O   | 1.88                     | 0.68              |
| 58:BZ:44:PHE:CZ    | 58:BZ:48:PHE:HD2  | 2.11                     | 0.68              |
| 1:AA:1218:C:H2'    | 1:AA:1219:U:C6    | 2.28                     | 0.68              |
| 1:AA:1305:G:N2     | 1:AA:1331:G:H2'   | 2.09                     | 0.68              |
| 1:AA:1402:C:C2'    | 1:AA:1403:C:H5'   | 2.23                     | 0.68              |
| 1:AA:46:G:HO2'     | 1:AA:365:U:C1'    | 2.06                     | 0.68              |
| 1:AA:88:A:H5''     | 1:AA:89:C:OP1     | 1.93                     | 0.68              |
| 12:AL:93:LEU:HB3   | 12:AL:96:VAL:HG21 | 1.76                     | 0.68              |
| 30:B5:16:ARG:NH1   | 30:B5:17:ASP:OD1  | 2.26                     | 0.68              |
| 31:B6:43:CYS:O     | 31:B6:44:ARG:HB2  | 1.92                     | 0.68              |
| 35:BA:2007:C:H2'   | 35:BA:2008:C:C6   | 2.28                     | 0.68              |
| 35:BA:2208:A:H1'   | 35:BA:2219:G:C4   | 2.28                     | 0.68              |
| 35:BA:2783:G:H2'   | 35:BA:2784:C:C6   | 2.28                     | 0.68              |
| 35:BA:697:C:O2'    | 35:BA:698:C:C5'   | 2.30                     | 0.68              |
| 37:BC:46:ALA:HB3   | 37:BC:172:ILE:CG2 | 2.23                     | 0.68              |
| 52:BT:3:ARG:HD2    | 52:BT:6:LEU:HB2   | 1.75                     | 0.68              |
| 2:AB:145:LEU:CD2   | 2:AB:149:LEU:HD23 | 2.23                     | 0.68              |
| 7:AG:38:LEU:O      | 7:AG:38:LEU:HD22  | 1.93                     | 0.68              |
| 30:B5:44:THR:CG2   | 50:BR:101:ALA:HB2 | 2.23                     | 0.68              |
| 35:BA:1461:G:C2'   | 35:BA:1462:C:H5'  | 2.24                     | 0.68              |
| 35:BA:175:G:C2'    | 35:BA:176:G:H5'   | 2.23                     | 0.68              |
| 35:BA:1821:A:O2'   | 35:BA:1822:G:C5'  | 2.39                     | 0.68              |
| 35:BA:1887:C:H2'   | 35:BA:1888:G:C5'  | 2.24                     | 0.68              |
| 39:BE:69:LYS:C     | 39:BE:71:GLY:H    | 1.96                     | 0.68              |
| 41:BG:94:LEU:HD12  | 41:BG:98:ARG:HD3  | 1.76                     | 0.68              |
| 49:BQ:12:GLN:CG    | 49:BQ:73:PRO:HD2  | 2.23                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:BR:38:VAL:HB    | 50:BR:39:PRO:HD3   | 1.76                     | 0.68              |
| 1:AA:593:G:O2'     | 1:AA:594:G:C5'     | 2.30                     | 0.68              |
| 12:AL:45:PRO:HG3   | 12:AL:53:ARG:HD3   | 1.75                     | 0.68              |
| 13:AM:108:ARG:HG3  | 13:AM:108:ARG:NH1  | 2.08                     | 0.68              |
| 27:B2:70:GLN:NE2   | 27:B2:71:ASN:N     | 2.42                     | 0.68              |
| 35:BA:1352:U:O2'   | 35:BA:1353:A:H5'   | 1.94                     | 0.68              |
| 35:BA:1646:C:H5''  | 35:BA:1647:G:C5'   | 2.24                     | 0.68              |
| 37:BC:123:ALA:O    | 37:BC:127:LYS:HG2  | 1.94                     | 0.68              |
| 37:BC:57:GLN:HG3   | 37:BC:57:GLN:O     | 1.93                     | 0.68              |
| 41:BG:37:VAL:HG21  | 41:BG:99:MET:HG3   | 1.76                     | 0.68              |
| 48:BP:29:LYS:HD2   | 48:BP:29:LYS:N     | 2.09                     | 0.68              |
| 25:B0:7:LEU:HB3    | 49:BQ:85:LYS:HG3   | 1.76                     | 0.68              |
| 51:BS:49:VAL:HG12  | 51:BS:50:SER:H     | 1.57                     | 0.68              |
| 52:BT:92:GLY:HA3   | 52:BT:120:ARG:HH21 | 1.59                     | 0.68              |
| 55:BW:64:MET:O     | 55:BW:65:LEU:HB2   | 1.92                     | 0.68              |
| 1:AA:198:G:C6      | 1:AA:220:G:C6      | 2.80                     | 0.68              |
| 1:AA:309:G:O2'     | 1:AA:310:G:H5'     | 1.94                     | 0.68              |
| 10:AJ:54:PHE:CE1   | 10:AJ:55:LYS:NZ    | 2.56                     | 0.68              |
| 1:AA:563:A:H2      | 12:AL:15:ARG:CZ    | 2.06                     | 0.68              |
| 12:AL:70:ILE:HG12  | 12:AL:100:ILE:HD12 | 1.74                     | 0.68              |
| 13:AM:118:ALA:HB1  | 19:AS:88:LYS:NZ    | 2.09                     | 0.68              |
| 24:AY:169:GLY:HA3  | 24:AY:173:THR:O    | 1.93                     | 0.68              |
| 29:B4:33:VAL:O     | 29:B4:34:GLU:HB2   | 1.94                     | 0.68              |
| 31:B6:12:GLU:CB    | 31:B6:23:THR:HG22  | 2.24                     | 0.68              |
| 35:BA:261:G:H2'    | 35:BA:262:A:H5'    | 1.76                     | 0.68              |
| 37:BC:176:VAL:HG11 | 37:BC:190:ILE:HD13 | 1.76                     | 0.68              |
| 37:BC:30:VAL:HG23  | 37:BC:31:LYS:N     | 2.09                     | 0.68              |
| 52:BT:109:GLU:O    | 52:BT:112:ARG:HG2  | 1.94                     | 0.68              |
| 52:BT:28:VAL:CG1   | 52:BT:29:ARG:N     | 2.54                     | 0.68              |
| 1:AA:490:G:C4      | 1:AA:491:G:N7      | 2.62                     | 0.67              |
| 1:AA:39:G:N7       | 1:AA:547:A:C8      | 2.62                     | 0.67              |
| 1:AA:35:G:N2       | 1:AA:549:C:O2      | 2.17                     | 0.67              |
| 19:AS:40:ILE:HG12  | 19:AS:66:MET:O     | 1.93                     | 0.67              |
| 25:B0:62:LEU:H     | 25:B0:62:LEU:HD23  | 1.59                     | 0.67              |
| 27:B2:48:HIS:C     | 27:B2:48:HIS:CD2   | 2.67                     | 0.67              |
| 30:B5:16:ARG:HD2   | 30:B5:20:ARG:NH1   | 2.10                     | 0.67              |
| 30:B5:40:LYS:HE2   | 30:B5:46:CYS:HB3   | 1.75                     | 0.67              |
| 31:B6:15:GLU:OE1   | 31:B6:18:ARG:NE    | 2.27                     | 0.67              |
| 35:BA:1415:U:O5'   | 35:BA:1415:U:H6    | 1.76                     | 0.67              |
| 35:BA:953:A:H2'    | 35:BA:954:G:C5'    | 2.13                     | 0.67              |
| 38:BD:241:PRO:O    | 38:BD:242:ARG:HB2  | 1.92                     | 0.67              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:107:G:C2'     | 1:AA:108:G:O5'    | 2.40                     | 0.67              |
| 1:AA:1504:G:H4'    | 1:AA:1505:G:O4'   | 1.93                     | 0.67              |
| 1:AA:495:A:H4'     | 1:AA:496:A:OP1    | 1.94                     | 0.67              |
| 1:AA:687:A:H4'     | 1:AA:688:G:O5'    | 1.94                     | 0.67              |
| 3:AC:22:TRP:HZ3    | 3:AC:24:ALA:HB2   | 1.58                     | 0.67              |
| 26:B1:59:THR:C     | 26:B1:60:PHE:CD1  | 2.67                     | 0.67              |
| 27:B2:70:GLN:HE21  | 27:B2:71:ASN:H    | 1.40                     | 0.67              |
| 29:B4:11:PRO:CB    | 29:B4:24:THR:HB   | 2.25                     | 0.67              |
| 26:B1:41:ARG:HH12  | 35:BA:1365:A:H5'' | 1.58                     | 0.67              |
| 35:BA:833:U:C4'    | 48:BP:52:GLU:N    | 2.56                     | 0.67              |
| 35:BA:900:A:H3'    | 35:BA:901:A:H8    | 1.58                     | 0.67              |
| 35:BA:967:C:O5'    | 35:BA:967:C:H6    | 1.77                     | 0.67              |
| 35:BA:2128:C:OP1   | 37:BC:37:LYS:HG2  | 1.94                     | 0.67              |
| 39:BE:197:ILE:HD11 | 39:BE:199:ARG:NE  | 2.09                     | 0.67              |
| 39:BE:24:THR:HG21  | 39:BE:188:VAL:CG1 | 2.23                     | 0.67              |
| 46:BN:1:MET:C      | 46:BN:2:LYS:HE3   | 2.13                     | 0.67              |
| 35:BA:2562:U:H1'   | 47:BO:23:ARG:HH11 | 1.58                     | 0.67              |
| 54:BV:2:PHE:C      | 54:BV:2:PHE:CD1   | 2.66                     | 0.67              |
| 57:BY:28:LYS:CB    | 57:BY:38:ILE:H    | 2.07                     | 0.67              |
| 3:AC:16:ARG:CD     | 3:AC:17:ASP:H     | 2.07                     | 0.67              |
| 29:B4:11:PRO:CA    | 29:B4:24:THR:HB   | 2.24                     | 0.67              |
| 31:B6:6:ARG:NH1    | 31:B6:6:ARG:HB3   | 2.07                     | 0.67              |
| 35:BA:1446:C:C5    | 35:BA:1465:G:N2   | 2.59                     | 0.67              |
| 35:BA:1769:G:C5    | 35:BA:1984:G:C6   | 2.83                     | 0.67              |
| 35:BA:52:A:C2'     | 35:BA:53:A:H5'    | 2.23                     | 0.67              |
| 48:BP:14:LYS:O     | 48:BP:15:ARG:HB2  | 1.94                     | 0.67              |
| 48:BP:97:PRO:O     | 48:BP:98:GLU:HB3  | 1.94                     | 0.67              |
| 51:BS:36:TYR:HD1   | 51:BS:36:TYR:N    | 1.92                     | 0.67              |
| 1:AA:61:G:O6       | 1:AA:107:G:C6     | 2.48                     | 0.67              |
| 2:AB:42:ILE:CD1    | 2:AB:202:PRO:HB2  | 2.25                     | 0.67              |
| 3:AC:129:ALA:HB1   | 3:AC:132:ARG:HG3  | 1.76                     | 0.67              |
| 6:AF:99:ALA:O      | 6:AF:100:ASN:HB2  | 1.93                     | 0.67              |
| 17:AQ:67:LYS:HA    | 17:AQ:70:ARG:NH1  | 2.08                     | 0.67              |
| 26:B1:25:LYS:HD3   | 35:BA:2396:G:C5'  | 2.24                     | 0.67              |
| 33:B8:15:LYS:CD    | 48:BP:65:ARG:HH22 | 2.07                     | 0.67              |
| 35:BA:1028:A:H2'   | 35:BA:1029:A:C8   | 2.30                     | 0.67              |
| 35:BA:2007:C:C2    | 35:BA:2008:C:C5   | 2.82                     | 0.67              |
| 35:BA:2103:C:H42   | 35:BA:2186:G:H1   | 1.41                     | 0.67              |
| 35:BA:2657:A:H2'   | 35:BA:2658:C:H5'  | 1.76                     | 0.67              |
| 35:BA:37:C:C2'     | 35:BA:38:A:H5'    | 2.24                     | 0.67              |
| 35:BA:461:C:H2'    | 35:BA:462:C:C5'   | 2.14                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:603:A:H4'    | 35:BA:604:G:O5'    | 1.94                     | 0.67              |
| 40:BF:52:LYS:O     | 40:BF:88:VAL:HG12  | 1.95                     | 0.67              |
| 42:BH:54:ARG:HH11  | 42:BH:65:HIS:CD2   | 2.13                     | 0.67              |
| 50:BR:2:ARG:HG3    | 50:BR:2:ARG:NH1    | 2.05                     | 0.67              |
| 27:B2:40:SER:O     | 56:BX:13:LEU:CD1   | 2.43                     | 0.67              |
| 57:BY:17:SER:HB2   | 57:BY:71:LYS:HE2   | 1.75                     | 0.67              |
| 57:BY:82:PRO:O     | 57:BY:96:ILE:HG13  | 1.94                     | 0.67              |
| 1:AA:179:A:H2'     | 1:AA:180:U:H6      | 1.58                     | 0.67              |
| 1:AA:197:A:C4'     | 1:AA:198:G:O5'     | 2.34                     | 0.67              |
| 1:AA:36:C:H2'      | 1:AA:37:U:C6       | 2.30                     | 0.67              |
| 14:AN:15:LYS:O     | 14:AN:16:PHE:O     | 2.13                     | 0.67              |
| 35:BA:1902:C:H5'   | 38:BD:246:PRO:HD3  | 1.76                     | 0.67              |
| 35:BA:2033:A:H2'   | 35:BA:2035:G:OP2   | 1.95                     | 0.67              |
| 37:BC:30:VAL:HG23  | 37:BC:31:LYS:H     | 1.58                     | 0.67              |
| 37:BC:46:ALA:HB3   | 37:BC:172:ILE:HG22 | 1.75                     | 0.67              |
| 41:BG:152:LEU:HD23 | 41:BG:152:LEU:H    | 1.60                     | 0.67              |
| 1:AA:37:U:H6       | 1:AA:37:U:O5'      | 1.78                     | 0.67              |
| 1:AA:687:A:C4'     | 1:AA:688:G:O5'     | 2.43                     | 0.67              |
| 1:AA:792:A:C1'     | 1:AA:793:U:OP2     | 2.43                     | 0.67              |
| 4:AD:120:LEU:HB3   | 4:AD:126:ILE:HD11  | 1.75                     | 0.67              |
| 5:AE:31:LEU:CD2    | 5:AE:43:LEU:HD11   | 2.21                     | 0.67              |
| 9:AI:26:VAL:CG2    | 9:AI:61:ALA:O      | 2.27                     | 0.67              |
| 13:AM:64:TRP:HD1   | 13:AM:66:LEU:HD11  | 1.59                     | 0.67              |
| 25:B0:46:LYS:HE3   | 25:B0:75:LEU:O     | 1.92                     | 0.67              |
| 35:BA:1446:C:C5    | 35:BA:1466:G:C2    | 2.83                     | 0.67              |
| 35:BA:285:C:H2'    | 35:BA:286:C:H6     | 1.60                     | 0.67              |
| 35:BA:36:G:C2'     | 35:BA:37:C:H5'     | 2.25                     | 0.67              |
| 40:BF:20:LEU:H     | 40:BF:24:LEU:HD23  | 1.57                     | 0.67              |
| 41:BG:59:GLU:CG    | 41:BG:60:LEU:H     | 2.06                     | 0.67              |
| 50:BR:10:LEU:N     | 50:BR:10:LEU:HD23  | 2.09                     | 0.67              |
| 54:BV:61:VAL:O     | 54:BV:61:VAL:HG23  | 1.94                     | 0.67              |
| 1:AA:274:A:O2'     | 1:AA:275:G:C8      | 2.48                     | 0.67              |
| 7:AG:81:GLY:O      | 23:AX:13:A:P       | 2.52                     | 0.67              |
| 24:AY:487:ILE:HD13 | 24:AY:487:ILE:H    | 1.59                     | 0.67              |
| 24:AY:539:ILE:HB   | 24:AY:540:PRO:HD3  | 1.76                     | 0.67              |
| 24:AY:92:ILE:O     | 24:AY:96:ARG:HG2   | 1.95                     | 0.67              |
| 29:B4:38:LYS:O     | 29:B4:38:LYS:HD2   | 1.95                     | 0.67              |
| 33:B8:23:VAL:CG1   | 33:B8:46:ARG:HH11  | 2.07                     | 0.67              |
| 33:B8:29:LYS:HD3   | 33:B8:44:LYS:CB    | 2.25                     | 0.67              |
| 35:BA:1270:C:H5''  | 35:BA:1271:G:O5'   | 1.94                     | 0.67              |
| 35:BA:2469:A:H2    | 35:BA:2481:G:H21   | 1.40                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:BG:24:GLY:O    | 41:BG:25:TYR:HB2   | 1.95                     | 0.67              |
| 42:BH:9:ILE:HG22  | 42:BH:10:PRO:C     | 2.15                     | 0.67              |
| 42:BH:143:GLN:NE2 | 42:BH:147:ASN:HD21 | 1.92                     | 0.67              |
| 1:AA:1052:U:O4    | 1:AA:1200:C:C2'    | 2.39                     | 0.67              |
| 6:AF:67:MET:HB2   | 6:AF:68:PRO:HD2    | 1.76                     | 0.67              |
| 7:AG:115:ARG:O    | 7:AG:119:ARG:HD3   | 1.94                     | 0.67              |
| 7:AG:111:ARG:NH2  | 7:AG:126:ASP:OD2   | 2.28                     | 0.67              |
| 16:AP:22:THR:HA   | 16:AP:33:ILE:HG12  | 1.76                     | 0.67              |
| 24:AY:42:ILE:HG22 | 24:AY:44:GLU:H     | 1.60                     | 0.67              |
| 35:BA:1358:G:O2'  | 35:BA:1359:A:H5''  | 1.94                     | 0.67              |
| 35:BA:1858:G:H2'  | 35:BA:1883:G:H22   | 1.60                     | 0.67              |
| 35:BA:1926:U:H2'  | 35:BA:1927:A:C8    | 2.29                     | 0.67              |
| 35:BA:39:C:H6     | 35:BA:39:C:O5'     | 1.76                     | 0.67              |
| 1:AA:547:A:C1'    | 1:AA:548:G:OP2     | 2.40                     | 0.67              |
| 12:AL:27:LEU:O    | 12:AL:29:GLY:N     | 2.28                     | 0.67              |
| 14:AN:15:LYS:HB3  | 14:AN:16:PHE:CE1   | 2.30                     | 0.67              |
| 1:AA:235:C:H5'    | 17:AQ:70:ARG:HG2   | 1.76                     | 0.67              |
| 24:AY:358:MET:SD  | 24:AY:363:ARG:HD3  | 2.34                     | 0.67              |
| 24:AY:423:LYS:HD3 | 24:AY:472:VAL:HG22 | 1.77                     | 0.67              |
| 26:B1:82:LEU:O    | 26:B1:83:GLU:HG3   | 1.94                     | 0.67              |
| 29:B4:1:MET:O     | 29:B4:2:LYS:HB3    | 1.94                     | 0.67              |
| 35:BA:1773:A:C2'  | 35:BA:1774:C:C5'   | 2.62                     | 0.67              |
| 35:BA:2345:G:N3   | 35:BA:2381:C:H2'   | 2.10                     | 0.67              |
| 35:BA:2403:C:P    | 35:BA:2403:C:H3'   | 2.34                     | 0.67              |
| 35:BA:893:C:H2'   | 35:BA:894:C:C6     | 2.29                     | 0.67              |
| 35:BA:902:C:H2'   | 35:BA:903:C:C6     | 2.29                     | 0.67              |
| 39:BE:134:ILE:C   | 39:BE:134:ILE:HD12 | 2.14                     | 0.67              |
| 36:BB:43:C:H4'    | 41:BG:94:LEU:HD11  | 1.77                     | 0.67              |
| 43:BJ:72:UNK:O    | 43:BJ:74:UNK:N     | 2.28                     | 0.67              |
| 48:BP:71:VAL:CG1  | 48:BP:72:PRO:HD3   | 2.24                     | 0.67              |
| 49:BQ:43:THR:OG1  | 49:BQ:46:GLN:HG3   | 1.94                     | 0.67              |
| 54:BV:52:VAL:CG1  | 54:BV:55:ALA:HB3   | 2.24                     | 0.67              |
| 55:BW:36:LEU:H    | 55:BW:36:LEU:HD22  | 1.59                     | 0.67              |
| 1:AA:64:G:H4'     | 1:AA:65:U:O5'      | 1.95                     | 0.67              |
| 15:AO:68:ARG:NH1  | 15:AO:68:ARG:HB2   | 2.03                     | 0.67              |
| 24:AY:26:THR:CG2  | 24:AY:52:MET:HG2   | 2.25                     | 0.67              |
| 35:BA:1331:A:O2'  | 35:BA:1332:G:H5''  | 1.95                     | 0.67              |
| 35:BA:2157:G:H4'  | 35:BA:2158:A:OP1   | 1.95                     | 0.67              |
| 37:BC:133:GLY:C   | 37:BC:135:ARG:H    | 1.98                     | 0.67              |
| 49:BQ:140:ALA:HB1 | 58:BZ:99:TYR:CE2   | 2.30                     | 0.67              |
| 55:BW:37:ARG:HH11 | 55:BW:37:ARG:HG3   | 1.59                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1160:G:O6    | 1:AA:1181:G:O6     | 2.13                     | 0.66              |
| 1:AA:116:A:C8     | 1:AA:116:A:OP2     | 2.47                     | 0.66              |
| 1:AA:1255:G:C6    | 1:AA:1283:G:O6     | 2.48                     | 0.66              |
| 1:AA:1490:C:H2'   | 1:AA:1491:G:C5'    | 2.09                     | 0.66              |
| 1:AA:321:A:C2'    | 1:AA:322:C:H5'     | 2.24                     | 0.66              |
| 3:AC:116:VAL:HG11 | 3:AC:202:ILE:HD11  | 1.77                     | 0.66              |
| 9:AI:19:LEU:HA    | 9:AI:61:ALA:HA     | 1.75                     | 0.66              |
| 29:B4:30:GLU:HG2  | 29:B4:31:ILE:N     | 2.08                     | 0.66              |
| 35:BA:1646:C:C5'  | 35:BA:1647:G:C5'   | 2.73                     | 0.66              |
| 35:BA:1770:G:C2'  | 35:BA:1771:C:C5'   | 2.73                     | 0.66              |
| 35:BA:1890:A:C2'  | 35:BA:1891:G:C5'   | 2.66                     | 0.66              |
| 35:BA:1892:C:H2'  | 35:BA:1893:C:C5'   | 2.23                     | 0.66              |
| 35:BA:49:A:O2'    | 35:BA:50:U:P       | 2.53                     | 0.66              |
| 35:BA:942:G:H5'   | 48:BP:35:HIS:HA    | 1.76                     | 0.66              |
| 41:BG:136:ARG:HB3 | 41:BG:138:GLN:OE1  | 1.94                     | 0.66              |
| 42:BH:149:ARG:HA  | 42:BH:162:ILE:CD1  | 2.24                     | 0.66              |
| 1:AA:1399:C:H4'   | 1:AA:1400:C:C5'    | 2.25                     | 0.66              |
| 1:AA:185:A:O2'    | 1:AA:186:C:H5'     | 1.95                     | 0.66              |
| 1:AA:961:U:O2'    | 1:AA:962:C:C5'     | 2.44                     | 0.66              |
| 3:AC:91:LEU:HB3   | 3:AC:99:VAL:HG21   | 1.77                     | 0.66              |
| 7:AG:43:PHE:O     | 7:AG:46:ALA:HB3    | 1.95                     | 0.66              |
| 13:AM:17:VAL:HG22 | 13:AM:27:LYS:HE3   | 1.77                     | 0.66              |
| 13:AM:65:LYS:HB2  | 13:AM:69:GLU:HG2   | 1.77                     | 0.66              |
| 16:AP:20:VAL:HG23 | 16:AP:34:GLU:O     | 1.93                     | 0.66              |
| 26:B1:82:LEU:O    | 26:B1:83:GLU:CG    | 2.43                     | 0.66              |
| 31:B6:7:ILE:CG2   | 31:B6:27:LYS:HZ2   | 2.01                     | 0.66              |
| 35:BA:1600:C:HO2' | 35:BA:1601:G:H5'   | 1.57                     | 0.66              |
| 35:BA:1886:C:O2'  | 35:BA:1887:C:H5'   | 1.95                     | 0.66              |
| 35:BA:2117:A:O2'  | 35:BA:2118:U:H3'   | 1.95                     | 0.66              |
| 35:BA:2552:U:H6   | 35:BA:2552:U:O5'   | 1.78                     | 0.66              |
| 26:B1:76:ARG:HD2  | 35:BA:271(R):G:OP1 | 1.96                     | 0.66              |
| 35:BA:607:U:C4    | 35:BA:620:G:C5     | 2.83                     | 0.66              |
| 37:BC:31:LYS:NZ   | 37:BC:180:SER:O    | 2.28                     | 0.66              |
| 38:BD:35:LYS:C    | 38:BD:35:LYS:HZ2   | 1.99                     | 0.66              |
| 36:BB:56:G:H5'    | 41:BG:27:ASN:ND2   | 2.10                     | 0.66              |
| 1:AA:1062:U:H2'   | 1:AA:1063:C:C6     | 2.29                     | 0.66              |
| 1:AA:46:G:HO2'    | 1:AA:365:U:C2'     | 2.07                     | 0.66              |
| 9:AI:69:GLY:O     | 9:AI:73:GLN:HG3    | 1.94                     | 0.66              |
| 10:AJ:43:ARG:HG3  | 10:AJ:43:ARG:HH11  | 1.61                     | 0.66              |
| 11:AK:21:ILE:HD13 | 11:AK:82:VAL:HG23  | 1.78                     | 0.66              |
| 35:BA:1019:U:HO2' | 35:BA:1021:A:H2    | 1.40                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:1105:U:O2'  | 35:BA:1106:G:H5'   | 1.95                     | 0.66              |
| 35:BA:1416:G:C2   | 35:BA:1417:C:N3    | 2.64                     | 0.66              |
| 35:BA:1799:G:C1'  | 35:BA:1800:C:OP2   | 2.43                     | 0.66              |
| 35:BA:688:U:H6    | 35:BA:688:U:O5'    | 1.78                     | 0.66              |
| 35:BA:2334:G:H21  | 51:BS:18:ILE:HG12  | 1.60                     | 0.66              |
| 35:BA:1151:G:H5'' | 53:BU:81:HIS:CE1   | 2.30                     | 0.66              |
| 55:BW:9:TYR:H     | 55:BW:102:HIS:CD2  | 2.11                     | 0.66              |
| 1:AA:532:A:N1     | 3:AC:193:TYR:HB3   | 2.11                     | 0.66              |
| 2:AB:24:TRP:CE3   | 2:AB:32:ILE:HD11   | 2.31                     | 0.66              |
| 2:AB:76:GLN:O     | 2:AB:77:ALA:HB2    | 1.94                     | 0.66              |
| 2:AB:7:VAL:O      | 2:AB:11:LEU:HB2    | 1.95                     | 0.66              |
| 24:AY:84:THR:CG2  | 24:AY:85:PRO:N     | 2.57                     | 0.66              |
| 25:B0:25:ARG:HB2  | 25:B0:37:LEU:HD12  | 1.77                     | 0.66              |
| 35:BA:1221:C:H2'  | 35:BA:1221(A):C:H6 | 1.59                     | 0.66              |
| 35:BA:1412:A:H2'  | 35:BA:1413:G:H5'   | 1.76                     | 0.66              |
| 35:BA:2145:C:H5'  | 35:BA:2146:C:C5    | 2.30                     | 0.66              |
| 35:BA:2195:C:O2'  | 35:BA:2196:C:H5'   | 1.96                     | 0.66              |
| 35:BA:2401:U:H2'  | 35:BA:2402:C:OP1   | 1.95                     | 0.66              |
| 35:BA:741:G:H2'   | 35:BA:742:G:H5'    | 1.75                     | 0.66              |
| 37:BC:65:LEU:HB3  | 37:BC:189:ASN:ND2  | 2.11                     | 0.66              |
| 39:BE:76:ARG:HG3  | 39:BE:195:LEU:HD22 | 1.76                     | 0.66              |
| 41:BG:72:ARG:HA   | 41:BG:87:PRO:O     | 1.95                     | 0.66              |
| 48:BP:64:LYS:O    | 48:BP:65:ARG:C     | 2.34                     | 0.66              |
| 1:AA:1386:G:H2'   | 1:AA:1387:G:H5'    | 1.76                     | 0.66              |
| 1:AA:1401:G:N2    | 1:AA:1501:C:O2     | 2.18                     | 0.66              |
| 1:AA:722:A:N3     | 1:AA:722:A:H2'     | 2.08                     | 0.66              |
| 5:AE:10:MET:SD    | 5:AE:10:MET:N      | 2.69                     | 0.66              |
| 13:AM:27:LYS:HG3  | 13:AM:31:LYS:HE3   | 1.76                     | 0.66              |
| 13:AM:45:VAL:HG13 | 13:AM:48:LEU:HD12  | 1.77                     | 0.66              |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CB    | 2.26                     | 0.66              |
| 31:B6:10:LEU:HD12 | 33:B8:34:TRP:HB2   | 1.76                     | 0.66              |
| 35:BA:1058:G:C2'  | 35:BA:1059:G:H5''  | 2.24                     | 0.66              |
| 35:BA:2845:G:O2'  | 35:BA:2846:G:H5'   | 1.95                     | 0.66              |
| 35:BA:36:G:H2'    | 35:BA:37:C:H5'     | 1.76                     | 0.66              |
| 35:BA:607:U:C4    | 35:BA:620:G:C4     | 2.82                     | 0.66              |
| 35:BA:650:C:C3'   | 35:BA:651:G:H5''   | 2.24                     | 0.66              |
| 37:BC:63:VAL:O    | 37:BC:161:ARG:HA   | 1.96                     | 0.66              |
| 47:BO:66:LYS:H    | 47:BO:82:ASN:ND2   | 1.94                     | 0.66              |
| 51:BS:14:VAL:HG12 | 51:BS:15:ARG:N     | 2.10                     | 0.66              |
| 52:BT:91:ARG:HA   | 52:BT:116:ALA:HA   | 1.78                     | 0.66              |
| 1:AA:699:C:O2'    | 1:AA:700:G:H5'     | 1.94                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:748:C:H1'     | 1:AA:749:C:H5      | 1.61                     | 0.66              |
| 1:AA:774:G:C2'     | 1:AA:775:G:H5'     | 2.25                     | 0.66              |
| 1:AA:975:A:C8      | 1:AA:975:A:H5'     | 2.28                     | 0.66              |
| 27:B2:42:GLY:O     | 27:B2:43:GLN:C     | 2.34                     | 0.66              |
| 35:BA:1222:C:C2'   | 35:BA:1223:G:C5'   | 2.72                     | 0.66              |
| 35:BA:1587:A:H3'   | 35:BA:1588:C:H6    | 1.60                     | 0.66              |
| 40:BF:155:LEU:HD11 | 40:BF:176:LEU:HD13 | 1.76                     | 0.66              |
| 41:BG:147:ASP:O    | 41:BG:149:VAL:HG13 | 1.95                     | 0.66              |
| 52:BT:16:ARG:CB    | 52:BT:16:ARG:HH11  | 2.07                     | 0.66              |
| 1:AA:522:C:C2'     | 1:AA:523:A:C5'     | 2.74                     | 0.66              |
| 1:AA:792:A:C4'     | 1:AA:793:U:O5'     | 2.41                     | 0.66              |
| 8:AH:89:PRO:HA     | 8:AH:92:ARG:NH1    | 2.06                     | 0.66              |
| 1:AA:522:C:N4      | 12:AL:53:ARG:HH22  | 1.92                     | 0.66              |
| 24:AY:228:MET:O    | 24:AY:231:TYR:HB3  | 1.96                     | 0.66              |
| 24:AY:44:GLU:O     | 24:AY:45:VAL:HG22  | 1.96                     | 0.66              |
| 24:AY:685:GLU:HA   | 24:AY:688:ILE:HD13 | 1.78                     | 0.66              |
| 35:BA:1782:C:H1'   | 35:BA:2609:U:H5'   | 1.78                     | 0.66              |
| 35:BA:2006:C:C4    | 35:BA:2007:C:N4    | 2.64                     | 0.66              |
| 35:BA:2033:A:O2'   | 35:BA:2034:U:P     | 2.54                     | 0.66              |
| 35:BA:259:G:H21    | 35:BA:621:A:H8     | 1.43                     | 0.66              |
| 35:BA:833:U:H4'    | 48:BP:51:PHE:O     | 1.96                     | 0.66              |
| 36:BB:48:A:H4'     | 51:BS:95:HIS:HD2   | 1.60                     | 0.66              |
| 42:BH:159:GLU:HA   | 42:BH:159:GLU:OE1  | 1.96                     | 0.66              |
| 35:BA:943:U:OP2    | 48:BP:38:GLN:CD    | 2.34                     | 0.66              |
| 52:BT:29:ARG:C     | 52:BT:30:VAL:HG23  | 2.15                     | 0.66              |
| 1:AA:346:G:C5'     | 52:BT:35:LYS:HZ1   | 2.09                     | 0.66              |
| 1:AA:917:G:O2'     | 1:AA:918:A:H5'     | 1.96                     | 0.66              |
| 14:AN:15:LYS:HB3   | 14:AN:16:PHE:CD1   | 2.30                     | 0.66              |
| 24:AY:114:VAL:HG23 | 24:AY:152:THR:HG23 | 1.76                     | 0.66              |
| 24:AY:199:ILE:O    | 24:AY:199:ILE:HD12 | 1.95                     | 0.66              |
| 34:B9:17:ILE:HG22  | 34:B9:18:ARG:N     | 2.10                     | 0.66              |
| 35:BA:110:G:H2'    | 35:BA:111:A:H5'    | 1.76                     | 0.66              |
| 35:BA:1273:U:H5''  | 35:BA:1646:C:H41   | 1.60                     | 0.66              |
| 35:BA:2408:U:H2'   | 35:BA:2409:G:C8    | 2.30                     | 0.66              |
| 35:BA:2656:U:H2'   | 35:BA:2657:A:H5''  | 1.77                     | 0.66              |
| 35:BA:49:A:P       | 35:BA:51:G:H5'     | 2.36                     | 0.66              |
| 35:BA:674:G:H1'    | 40:BF:74:ARG:HD2   | 1.78                     | 0.66              |
| 35:BA:952:G:C6     | 35:BA:953:A:N7     | 2.64                     | 0.66              |
| 39:BE:111:ARG:HG3  | 39:BE:160:TYR:CD2  | 2.31                     | 0.66              |
| 41:BG:7:LEU:C      | 41:BG:7:LEU:HD23   | 2.16                     | 0.66              |
| 42:BH:44:VAL:HG12  | 42:BH:46:GLU:H     | 1.61                     | 0.66              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 52:BT:19:LEU:HD22   | 52:BT:85:LYS:HB2    | 1.78                     | 0.66              |
| 1:AA:1003:G:H2'     | 1:AA:1004:A:O4'     | 1.96                     | 0.66              |
| 1:AA:939:G:N2       | 1:AA:1344:C:N3      | 2.42                     | 0.66              |
| 19:AS:62:ILE:HA     | 19:AS:66:MET:CE     | 2.26                     | 0.66              |
| 27:B2:5:GLU:HA      | 27:B2:8:LYS:CD      | 2.25                     | 0.66              |
| 35:BA:176:G:O2'     | 35:BA:177:G:C5'     | 2.44                     | 0.66              |
| 35:BA:1982:C:N4     | 35:BA:1983:C:N4     | 2.44                     | 0.66              |
| 37:BC:41:THR:O      | 37:BC:42:VAL:HB     | 1.94                     | 0.66              |
| 41:BG:117:PHE:CD2   | 41:BG:118:ARG:HD3   | 2.31                     | 0.66              |
| 41:BG:124:SER:HB3   | 41:BG:131:TYR:CE1   | 2.31                     | 0.66              |
| 35:BA:2305:A:C6     | 41:BG:137:GLU:OE2   | 2.49                     | 0.66              |
| 41:BG:39:ILE:HD11   | 41:BG:155:MET:CG    | 2.26                     | 0.66              |
| 49:BQ:1:MET:CE      | 49:BQ:1:MET:HA      | 2.26                     | 0.66              |
| 50:BR:87:TYR:O      | 50:BR:89:ASP:N      | 2.27                     | 0.66              |
| 53:BU:85:LYS:HD3    | 53:BU:117:GLN:NE2   | 2.10                     | 0.66              |
| 1:AA:1370:G:C2'     | 1:AA:1371:G:H5'     | 2.26                     | 0.66              |
| 1:AA:344:A:H4'      | 1:AA:345:C:OP1      | 1.94                     | 0.66              |
| 11:AK:126:ARG:NH1   | 11:AK:126:ARG:HB3   | 2.11                     | 0.66              |
| 35:BA:108:U:H2'     | 35:BA:109:G:H8      | 1.61                     | 0.66              |
| 35:BA:144:C:H2'     | 35:BA:145:G:C8      | 2.31                     | 0.66              |
| 35:BA:1961:C:O5'    | 35:BA:1961:C:H6     | 1.79                     | 0.66              |
| 35:BA:2131:G:OP1    | 35:BA:2132:U:H5''   | 1.96                     | 0.66              |
| 35:BA:271(L):U:H5'' | 35:BA:271(M):G:C5'  | 2.25                     | 0.66              |
| 35:BA:271(M):G:H2'  | 35:BA:271(N):U:H5'' | 1.78                     | 0.66              |
| 37:BC:42:VAL:HG13   | 37:BC:43:GLU:N      | 2.10                     | 0.66              |
| 48:BP:6:LEU:H       | 48:BP:6:LEU:HD23    | 1.60                     | 0.66              |
| 49:BQ:141:GLN:H     | 58:BZ:53:ILE:HD12   | 1.61                     | 0.66              |
| 57:BY:2:ARG:HD3     | 57:BY:3:VAL:HG23    | 1.78                     | 0.66              |
| 57:BY:13:VAL:HG21   | 57:BY:72:VAL:HB     | 1.77                     | 0.66              |
| 1:AA:113:G:H2'      | 1:AA:114:U:C6       | 2.31                     | 0.65              |
| 12:AL:17:LYS:CD     | 12:AL:18:VAL:H      | 2.08                     | 0.65              |
| 35:BA:1375:C:O2'    | 35:BA:1376:C:C5'    | 2.38                     | 0.65              |
| 35:BA:2123:G:C6     | 35:BA:2176:A:N6     | 2.64                     | 0.65              |
| 35:BA:2401:U:O2'    | 35:BA:2402:C:P      | 2.54                     | 0.65              |
| 35:BA:2422:A:H4'    | 35:BA:2423:U:OP1    | 1.96                     | 0.65              |
| 35:BA:247:G:C2'     | 35:BA:248:G:O5'     | 2.44                     | 0.65              |
| 35:BA:2611:U:H6     | 35:BA:2611:U:OP2    | 1.79                     | 0.65              |
| 35:BA:48:G:H2'      | 35:BA:49:A:H2       | 1.61                     | 0.65              |
| 35:BA:535:C:O2'     | 35:BA:536:A:H5'     | 1.96                     | 0.65              |
| 37:BC:129:GLY:O     | 37:BC:132:LEU:N     | 2.29                     | 0.65              |
| 40:BF:10:PRO:HA     | 40:BF:127:GLU:HG2   | 1.78                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:94:LEU:HD12  | 41:BG:98:ARG:HD2   | 1.77                     | 0.65              |
| 49:BQ:134:ARG:HA   | 49:BQ:137:TYR:HD2  | 1.60                     | 0.65              |
| 52:BT:28:VAL:HG11  | 52:BT:46:GLU:HG3   | 1.76                     | 0.65              |
| 1:AA:1195:C:H6     | 1:AA:1195:C:O5'    | 1.79                     | 0.65              |
| 3:AC:173:VAL:O     | 3:AC:173:VAL:HG13  | 1.94                     | 0.65              |
| 3:AC:187:ALA:HB3   | 3:AC:198:VAL:HB    | 1.77                     | 0.65              |
| 10:AJ:66:ARG:HH11  | 10:AJ:66:ARG:HB2   | 1.60                     | 0.65              |
| 12:AL:41:ARG:O     | 12:AL:55:VAL:O     | 2.14                     | 0.65              |
| 12:AL:24:VAL:HG13  | 12:AL:98:TYR:HE2   | 1.61                     | 0.65              |
| 24:AY:137:ASN:ND2  | 24:AY:138:LYS:N    | 2.42                     | 0.65              |
| 24:AY:627:ARG:O    | 24:AY:628:ARG:HB2  | 1.96                     | 0.65              |
| 35:BA:1797:C:O5'   | 35:BA:1797:C:H6    | 1.79                     | 0.65              |
| 35:BA:2103:C:O2'   | 35:BA:2104:G:H5'   | 1.96                     | 0.65              |
| 35:BA:2134:A:C8    | 35:BA:2158:A:H2    | 2.14                     | 0.65              |
| 35:BA:2356:C:C2'   | 35:BA:2357:U:O5'   | 2.43                     | 0.65              |
| 35:BA:2392:A:H2    | 35:BA:2424:C:N4    | 1.94                     | 0.65              |
| 37:BC:144:GLY:C    | 37:BC:161:ARG:HH21 | 1.99                     | 0.65              |
| 37:BC:206:LYS:HB3  | 37:BC:206:LYS:NZ   | 2.12                     | 0.65              |
| 37:BC:84:ILE:HG13  | 37:BC:84:ILE:O     | 1.95                     | 0.65              |
| 39:BE:87:GLU:O     | 39:BE:89:ASP:N     | 2.28                     | 0.65              |
| 47:BO:10:VAL:HG21  | 47:BO:16:ALA:O     | 1.96                     | 0.65              |
| 48:BP:112:LEU:HD23 | 48:BP:113:LYS:N    | 2.11                     | 0.65              |
| 58:BZ:183:LEU:HD13 | 58:BZ:183:LEU:C    | 2.15                     | 0.65              |
| 1:AA:1116:C:H2'    | 1:AA:1117:G:H5'    | 1.75                     | 0.65              |
| 1:AA:17:U:H2'      | 1:AA:18:C:C6       | 2.30                     | 0.65              |
| 1:AA:255:G:H1'     | 17:AQ:16:GLN:NE2   | 2.11                     | 0.65              |
| 1:AA:311:C:O2'     | 1:AA:312:C:H5''    | 1.96                     | 0.65              |
| 3:AC:123:GLN:HE22  | 3:AC:128:PHE:HB2   | 1.61                     | 0.65              |
| 24:AY:238:THR:CG2  | 24:AY:241:GLU:HG2  | 2.24                     | 0.65              |
| 31:B6:9:LEU:CD1    | 31:B6:9:LEU:C      | 2.63                     | 0.65              |
| 33:B8:4:MET:HG2    | 33:B8:61:LEU:HD23  | 1.77                     | 0.65              |
| 35:BA:2777:G:H5''  | 35:BA:2778:A:H5'   | 1.77                     | 0.65              |
| 36:BB:56:G:H4'     | 36:BB:57:A:O5'     | 1.96                     | 0.65              |
| 40:BF:24:LEU:HB3   | 40:BF:25:PRO:CD    | 2.24                     | 0.65              |
| 41:BG:75:LYS:HG2   | 41:BG:76:SER:N     | 2.10                     | 0.65              |
| 42:BH:12:PRO:HD3   | 42:BH:76:VAL:CG1   | 2.26                     | 0.65              |
| 57:BY:9:LYS:O      | 57:BY:28:LYS:HD3   | 1.96                     | 0.65              |
| 1:AA:112:G:O2'     | 1:AA:113:G:C5'     | 2.45                     | 0.65              |
| 1:AA:1384:C:O2'    | 1:AA:1385:G:H5'    | 1.96                     | 0.65              |
| 1:AA:1488:G:H2'    | 1:AA:1489:G:C8     | 2.31                     | 0.65              |
| 1:AA:56:U:O2'      | 1:AA:57:G:H5'      | 1.97                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:62:U:O5'     | 1:AA:62:U:H6       | 1.79                     | 0.65              |
| 3:AC:191:THR:HG22 | 3:AC:192:THR:N     | 2.12                     | 0.65              |
| 9:AI:71:SER:HA    | 9:AI:74:ILE:HD12   | 1.78                     | 0.65              |
| 17:AQ:68:ARG:H    | 17:AQ:70:ARG:HH11  | 1.45                     | 0.65              |
| 24:AY:252:ASP:HB3 | 24:AY:254:LYS:HZ2  | 1.59                     | 0.65              |
| 29:B4:32:TYR:O    | 29:B4:33:VAL:CG1   | 2.35                     | 0.65              |
| 35:BA:1025:G:C4   | 35:BA:1135:C:H1'   | 2.31                     | 0.65              |
| 35:BA:1990:C:H6   | 35:BA:1990:C:O5'   | 1.78                     | 0.65              |
| 25:B0:12:ASN:HB2  | 35:BA:2278:A:N7    | 2.11                     | 0.65              |
| 35:BA:2308:G:H2'  | 35:BA:2309:A:C8    | 2.31                     | 0.65              |
| 35:BA:2653:U:H5'' | 35:BA:2654:A:H2'   | 1.78                     | 0.65              |
| 35:BA:1653:G:OP1  | 35:BA:2822:G:N1    | 2.30                     | 0.65              |
| 35:BA:688:U:H2'   | 35:BA:689:A:H5'    | 1.76                     | 0.65              |
| 35:BA:702:G:C2'   | 35:BA:703:U:C5'    | 2.72                     | 0.65              |
| 35:BA:856:C:O2'   | 35:BA:857:C:P      | 2.54                     | 0.65              |
| 35:BA:971:C:H2'   | 35:BA:972:G:O4'    | 1.95                     | 0.65              |
| 39:BE:16:ARG:HH21 | 39:BE:173:VAL:HG13 | 1.62                     | 0.65              |
| 39:BE:51:PHE:CE2  | 39:BE:52:LEU:HD13  | 2.32                     | 0.65              |
| 42:BH:157:TYR:HE1 | 42:BH:171:LEU:HD22 | 1.61                     | 0.65              |
| 1:AA:39:G:H2'     | 1:AA:40:C:H5'      | 1.78                     | 0.65              |
| 9:AI:21:PRO:HA    | 9:AI:58:HIS:O      | 1.97                     | 0.65              |
| 12:AL:78:GLN:NE2  | 24:AY:444:PRO:HA   | 2.12                     | 0.65              |
| 13:AM:91:ARG:CB   | 13:AM:98:VAL:HG12  | 2.25                     | 0.65              |
| 15:AO:80:ALA:O    | 15:AO:84:LYS:HG3   | 1.97                     | 0.65              |
| 24:AY:282:SER:HB3 | 24:AY:285:ASP:OD1  | 1.97                     | 0.65              |
| 31:B6:35:GLU:H    | 31:B6:51:GLU:HG3   | 1.60                     | 0.65              |
| 35:BA:1062:G:H2'  | 35:BA:1063:G:C8    | 2.32                     | 0.65              |
| 35:BA:155:U:C2'   | 35:BA:156:U:H5''   | 2.23                     | 0.65              |
| 35:BA:49:A:N6     | 35:BA:177:G:N3     | 2.44                     | 0.65              |
| 35:BA:2000:G:N2   | 35:BA:2001:A:C5    | 2.65                     | 0.65              |
| 35:BA:332:A:C2    | 35:BA:335:C:C5     | 2.84                     | 0.65              |
| 35:BA:523:C:O2'   | 35:BA:524:U:C5'    | 2.31                     | 0.65              |
| 35:BA:743:G:O6    | 35:BA:755:C:N4     | 2.29                     | 0.65              |
| 37:BC:84:ILE:O    | 37:BC:86:GLU:N     | 2.30                     | 0.65              |
| 38:BD:43:ARG:CB   | 38:BD:54:ARG:HB2   | 2.26                     | 0.65              |
| 40:BF:125:LEU:H   | 40:BF:125:LEU:HD23 | 1.61                     | 0.65              |
| 40:BF:161:GLU:O   | 40:BF:165:ARG:HG3  | 1.96                     | 0.65              |
| 41:BG:83:ARG:N    | 41:BG:83:ARG:HD2   | 2.11                     | 0.65              |
| 35:BA:627:A:N6    | 48:BP:116:GLY:HA2  | 2.11                     | 0.65              |
| 48:BP:66:GLY:O    | 48:BP:67:MET:HB2   | 1.96                     | 0.65              |
| 56:BX:80:ILE:O    | 56:BX:80:ILE:HG12  | 1.97                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1026:G:N3     | 1:AA:1026:G:H2'   | 2.12                     | 0.65              |
| 1:AA:1304:G:H1'    | 1:AA:1333:A:H61   | 1.62                     | 0.65              |
| 1:AA:1492:A:H1'    | 1:AA:1493:A:P     | 2.35                     | 0.65              |
| 1:AA:193:C:O2'     | 1:AA:194:C:H5'    | 1.95                     | 0.65              |
| 1:AA:204:U:H2'     | 1:AA:204:U:O2     | 1.97                     | 0.65              |
| 1:AA:773:G:H2'     | 1:AA:774:G:C8     | 2.28                     | 0.65              |
| 3:AC:16:ARG:HH11   | 3:AC:16:ARG:HB2   | 1.61                     | 0.65              |
| 14:AN:58:LYS:NZ    | 14:AN:58:LYS:HB3  | 2.12                     | 0.65              |
| 16:AP:20:VAL:HG21  | 16:AP:32:TYR:HB2  | 1.78                     | 0.65              |
| 18:AR:26:LEU:HD21  | 18:AR:42:ARG:NH2  | 2.12                     | 0.65              |
| 24:AY:156:ARG:HH22 | 24:AY:666:ARG:NH1 | 1.93                     | 0.65              |
| 24:AY:683:VAL:O    | 24:AY:687:LEU:HG  | 1.96                     | 0.65              |
| 30:B5:51:TYR:O     | 30:B5:54:GLY:N    | 2.30                     | 0.65              |
| 35:BA:1983:C:H5''  | 35:BA:2607:G:OP1  | 1.95                     | 0.65              |
| 35:BA:2124:G:C2'   | 35:BA:2125:G:H5'  | 2.27                     | 0.65              |
| 35:BA:459:U:O2'    | 35:BA:460:A:H5'   | 1.95                     | 0.65              |
| 35:BA:742:G:HO2'   | 35:BA:743:G:H5''  | 1.60                     | 0.65              |
| 39:BE:132:HIS:HA   | 39:BE:135:HIS:HE1 | 1.57                     | 0.65              |
| 46:BN:120:LEU:HD13 | 46:BN:120:LEU:O   | 1.96                     | 0.65              |
| 54:BV:25:LEU:H     | 54:BV:92:THR:HG21 | 1.61                     | 0.65              |
| 1:AA:1148:U:H2'    | 1:AA:1149:C:C5'   | 2.27                     | 0.65              |
| 1:AA:1151:A:N3     | 1:AA:1152:A:N7    | 2.43                     | 0.65              |
| 1:AA:1151:A:N3     | 1:AA:1152:A:C5    | 2.64                     | 0.65              |
| 1:AA:509:A:C3'     | 1:AA:509:A:OP2    | 2.44                     | 0.65              |
| 2:AB:149:LEU:O     | 2:AB:151:GLY:N    | 2.30                     | 0.65              |
| 9:AI:23:ASN:N      | 9:AI:60:ASP:OD1   | 2.29                     | 0.65              |
| 20:AT:69:GLY:O     | 20:AT:73:HIS:CD2  | 2.49                     | 0.65              |
| 33:B8:33:ASN:CG    | 33:B8:34:TRP:N    | 2.50                     | 0.65              |
| 35:BA:1773:A:N7    | 35:BA:1829:A:C1'  | 2.60                     | 0.65              |
| 35:BA:2512:C:H2'   | 35:BA:2513:G:O4'  | 1.97                     | 0.65              |
| 41:BG:103:LEU:O    | 41:BG:104:GLU:HG2 | 1.96                     | 0.65              |
| 41:BG:145:THR:O    | 41:BG:146:TYR:O   | 2.15                     | 0.65              |
| 51:BS:54:LEU:HD21  | 51:BS:59:LYS:O    | 1.96                     | 0.65              |
| 57:BY:44:ILE:HG22  | 57:BY:45:VAL:N    | 2.11                     | 0.65              |
| 1:AA:1005:A:H2'    | 1:AA:1006:C:H5'   | 1.79                     | 0.65              |
| 1:AA:1255:G:O6     | 1:AA:1283:G:O6    | 2.15                     | 0.65              |
| 1:AA:179:A:H2'     | 1:AA:180:U:C6     | 2.31                     | 0.65              |
| 3:AC:64:VAL:HG12   | 3:AC:66:VAL:HG23  | 1.77                     | 0.65              |
| 12:AL:46:LYS:O     | 12:AL:47:LYS:C    | 2.35                     | 0.65              |
| 13:AM:116:THR:HG22 | 13:AM:117:VAL:H   | 1.61                     | 0.65              |
| 25:B0:19:LYS:HZ2   | 25:B0:41:ARG:HH22 | 1.45                     | 0.65              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:BA:1892:C:O5'   | 35:BA:1892:C:H6     | 1.79                     | 0.65              |
| 35:BA:1994:C:C2'   | 35:BA:1995:U:H5'    | 2.26                     | 0.65              |
| 35:BA:2104:G:H1'   | 35:BA:2105:C:P      | 2.36                     | 0.65              |
| 35:BA:2145:C:H4'   | 35:BA:2146:C:OP2    | 1.96                     | 0.65              |
| 35:BA:629:G:N1     | 35:BA:634:C:N3      | 2.43                     | 0.65              |
| 35:BA:769:G:H4'    | 35:BA:1379:A:C6     | 2.32                     | 0.65              |
| 42:BH:55:PRO:HG2   | 42:BH:56:SER:H      | 1.60                     | 0.65              |
| 51:BS:36:TYR:CD1   | 51:BS:36:TYR:N      | 2.64                     | 0.65              |
| 52:BT:96:ARG:HB2   | 52:BT:96:ARG:CZ     | 2.26                     | 0.65              |
| 54:BV:52:VAL:HG11  | 54:BV:55:ALA:HB3    | 1.79                     | 0.65              |
| 57:BY:98:VAL:HG12  | 57:BY:99:CYS:N      | 2.11                     | 0.65              |
| 1:AA:110:C:H2'     | 1:AA:111:G:H5'      | 1.79                     | 0.65              |
| 1:AA:1285:A:C4'    | 1:AA:1286:A:O5'     | 2.39                     | 0.65              |
| 1:AA:1526:G:C2'    | 1:AA:1527:C:H5'     | 2.26                     | 0.65              |
| 1:AA:189(L):G:H2'  | 1:AA:190:U:C6       | 2.32                     | 0.65              |
| 1:AA:1228:C:OP1    | 13:AM:115:LYS:HB2   | 1.96                     | 0.65              |
| 24:AY:99:ARG:HD3   | 24:AY:401:SER:CB    | 2.26                     | 0.65              |
| 31:B6:8:LYS:HG3    | 31:B6:26:ASN:O      | 1.96                     | 0.65              |
| 35:BA:272(H):C:H2' | 35:BA:272(I):U:H5'' | 1.79                     | 0.65              |
| 35:BA:28:A:H2'     | 35:BA:29:U:H5'      | 1.79                     | 0.65              |
| 37:BC:69:LEU:O     | 37:BC:178:LYS:HG3   | 1.97                     | 0.65              |
| 39:BE:117:MET:CE   | 39:BE:136:ARG:HA    | 2.27                     | 0.65              |
| 42:BH:5:GLY:N      | 42:BH:69:ARG:HD3    | 2.12                     | 0.65              |
| 1:AA:495:A:C2'     | 1:AA:496:A:H2'      | 2.27                     | 0.65              |
| 6:AF:4:TYR:HD1     | 6:AF:92:LYS:HA      | 1.60                     | 0.65              |
| 7:AG:12:LEU:HD13   | 7:AG:24:THR:HG22    | 1.80                     | 0.65              |
| 13:AM:15:VAL:HG11  | 13:AM:48:LEU:HD21   | 1.79                     | 0.65              |
| 26:B1:37:ILE:HD12  | 26:B1:37:ILE:C      | 2.17                     | 0.65              |
| 26:B1:82:LEU:C     | 26:B1:83:GLU:HG3    | 2.17                     | 0.65              |
| 29:B4:7:PRO:HG2    | 29:B4:9:LEU:CD1     | 2.26                     | 0.65              |
| 35:BA:267:C:O2'    | 35:BA:268:C:H5'     | 1.97                     | 0.65              |
| 35:BA:2779:U:H1'   | 35:BA:2781:A:C5     | 2.32                     | 0.65              |
| 35:BA:811:U:OP2    | 48:BP:33:ARG:NH1    | 2.30                     | 0.65              |
| 35:BA:856:C:C2'    | 35:BA:857:C:C6      | 2.63                     | 0.65              |
| 35:BA:944:G:H5'    | 35:BA:945:A:O5'     | 1.97                     | 0.65              |
| 35:BA:1902:C:H4'   | 38:BD:244:ARG:CA    | 2.26                     | 0.65              |
| 29:B4:7:PRO:HB3    | 41:BG:62:LEU:HG     | 1.78                     | 0.65              |
| 52:BT:34:VAL:HG22  | 52:BT:39:ARG:HB3    | 1.79                     | 0.65              |
| 52:BT:50:ILE:HA    | 52:BT:99:LEU:HD11   | 1.79                     | 0.65              |
| 52:BT:85:LYS:HZ3   | 52:BT:85:LYS:HB3    | 1.60                     | 0.65              |
| 1:AA:1237:C:HO2'   | 1:AA:1335:C:C4'     | 2.07                     | 0.64              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:1385:G:H2'     | 1:AA:1386:G:H8     | 1.61                     | 0.64              |
| 1:AA:64:G:H5'       | 1:AA:65:U:OP1      | 1.96                     | 0.64              |
| 1:AA:838:G:H2'      | 1:AA:839:U:H5''    | 1.79                     | 0.64              |
| 2:AB:200:ILE:CD1    | 2:AB:200:ILE:H     | 2.08                     | 0.64              |
| 3:AC:83:ARG:O       | 3:AC:85:ARG:N      | 2.30                     | 0.64              |
| 1:AA:738:C:H5''     | 6:AF:69:GLU:HB2    | 1.79                     | 0.64              |
| 2:AB:178:ARG:HH22   | 8:AH:68:ARG:HH12   | 1.45                     | 0.64              |
| 10:AJ:66:ARG:NH1    | 10:AJ:66:ARG:HB2   | 2.11                     | 0.64              |
| 12:AL:90:VAL:HG11   | 12:AL:93:LEU:HD12  | 1.77                     | 0.64              |
| 35:BA:2389:G:H5''   | 35:BA:2390:U:H5'   | 1.79                     | 0.64              |
| 39:BE:97:LYS:O      | 39:BE:100:GLU:HG3  | 1.97                     | 0.64              |
| 48:BP:78:PRO:HA     | 48:BP:110:TYR:CE2  | 2.32                     | 0.64              |
| 54:BV:67:GLY:O      | 54:BV:88:ARG:HD2   | 1.97                     | 0.64              |
| 1:AA:1216:G:O2'     | 1:AA:1217:C:H5'    | 1.98                     | 0.64              |
| 1:AA:545:C:O2'      | 1:AA:546:G:H5'     | 1.98                     | 0.64              |
| 2:AB:20:GLU:HB2     | 2:AB:190:THR:OG1   | 1.97                     | 0.64              |
| 2:AB:82:ARG:HB2     | 2:AB:92:TYR:OH     | 1.97                     | 0.64              |
| 4:AD:150:GLU:CG     | 4:AD:151:LYS:N     | 2.60                     | 0.64              |
| 24:AY:21:ILE:N      | 24:AY:21:ILE:HD12  | 2.12                     | 0.64              |
| 24:AY:401:SER:O     | 24:AY:402:ILE:HG13 | 1.97                     | 0.64              |
| 29:B4:34:GLU:O      | 29:B4:36:CYS:N     | 2.30                     | 0.64              |
| 35:BA:197:A:C8      | 35:BA:197:A:H5'    | 2.32                     | 0.64              |
| 35:BA:1992:G:H1'    | 35:BA:1993:U:OP2   | 1.96                     | 0.64              |
| 35:BA:271(Q):G:HO2' | 35:BA:271(R):G:H8  | 1.45                     | 0.64              |
| 35:BA:605:C:H2'     | 35:BA:606:U:C5'    | 2.27                     | 0.64              |
| 37:BC:102:GLN:O     | 37:BC:104:ILE:HG13 | 1.97                     | 0.64              |
| 37:BC:122:GLY:O     | 37:BC:127:LYS:HE3  | 1.96                     | 0.64              |
| 39:BE:36:ARG:NH2    | 39:BE:88:GLY:HA2   | 2.07                     | 0.64              |
| 42:BH:85:LYS:C      | 42:BH:85:LYS:HD3   | 2.18                     | 0.64              |
| 52:BT:29:ARG:NH1    | 52:BT:88:ILE:CD1   | 2.60                     | 0.64              |
| 53:BU:101:ARG:HH11  | 53:BU:101:ARG:HG3  | 1.61                     | 0.64              |
| 54:BV:51:VAL:HG12   | 54:BV:52:VAL:N     | 2.12                     | 0.64              |
| 58:BZ:119:GLU:HG3   | 58:BZ:122:ARG:HH12 | 1.62                     | 0.64              |
| 1:AA:1040:U:H2'     | 1:AA:1041:A:C8     | 2.32                     | 0.64              |
| 1:AA:1075:C:H2'     | 1:AA:1076:C:H5'    | 1.79                     | 0.64              |
| 1:AA:1153:C:O2'     | 1:AA:1154:G:P      | 2.55                     | 0.64              |
| 1:AA:362:G:N2       | 1:AA:365:U:OP2     | 2.30                     | 0.64              |
| 1:AA:589:C:H6       | 1:AA:589:C:O5'     | 1.79                     | 0.64              |
| 2:AB:218:ALA:O      | 2:AB:222:ILE:HG12  | 1.95                     | 0.64              |
| 24:AY:86:GLY:O      | 24:AY:117:GLN:CG   | 2.45                     | 0.64              |
| 24:AY:69:VAL:HB     | 24:AY:82:ILE:CD1   | 2.14                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:B8:52:LYS:H     | 33:B8:53:PRO:HD2   | 1.62                     | 0.64              |
| 35:BA:195:A:H5''   | 48:BP:46:LYS:HZ1   | 1.62                     | 0.64              |
| 35:BA:2469:A:C2'   | 35:BA:2470:G:H5'   | 2.27                     | 0.64              |
| 35:BA:2579:C:O3'   | 39:BE:131:ALA:HB2  | 1.97                     | 0.64              |
| 35:BA:2757:A:C2'   | 35:BA:2758:A:H5'   | 2.19                     | 0.64              |
| 35:BA:36:G:H4'     | 35:BA:451:C:C2     | 2.32                     | 0.64              |
| 48:BP:58:THR:O     | 48:BP:61:ARG:CD    | 2.45                     | 0.64              |
| 48:BP:61:ARG:C     | 48:BP:62:LEU:HD23  | 2.18                     | 0.64              |
| 50:BR:7:GLY:O      | 50:BR:8:ARG:HB2    | 1.97                     | 0.64              |
| 57:BY:42:VAL:HG21  | 57:BY:67:LEU:CD1   | 2.26                     | 0.64              |
| 1:AA:960:U:O2'     | 1:AA:1223:C:H4'    | 1.98                     | 0.64              |
| 1:AA:1390:U:H2'    | 1:AA:1391:U:H5'    | 1.78                     | 0.64              |
| 1:AA:46:G:O2'      | 1:AA:365:U:C2'     | 2.46                     | 0.64              |
| 2:AB:167:PRO:CG    | 2:AB:188:ALA:HB2   | 2.25                     | 0.64              |
| 3:AC:129:ALA:HB3   | 3:AC:133:ALA:HB2   | 1.79                     | 0.64              |
| 1:AA:408:A:H4'     | 4:AD:112:VAL:HG11  | 1.78                     | 0.64              |
| 6:AF:3:ARG:HB2     | 6:AF:3:ARG:CZ      | 2.25                     | 0.64              |
| 16:AP:28:ARG:HG2   | 16:AP:28:ARG:HH11  | 1.63                     | 0.64              |
| 21:AU:5:ASP:O      | 21:AU:11:GLY:HA3   | 1.97                     | 0.64              |
| 19:AS:67:VAL:HB    | 29:B4:50:VAL:HG13  | 1.79                     | 0.64              |
| 35:BA:1075:C:H2'   | 35:BA:1076:C:C6    | 2.31                     | 0.64              |
| 35:BA:1984:G:H2'   | 35:BA:1985:G:H5'   | 1.79                     | 0.64              |
| 35:BA:1984:G:HO2'  | 35:BA:1985:G:H5'   | 1.61                     | 0.64              |
| 35:BA:2105:C:C3'   | 35:BA:2106:G:H5''  | 2.27                     | 0.64              |
| 35:BA:962:G:H2'    | 35:BA:963:U:H5'    | 1.77                     | 0.64              |
| 37:BC:117:THR:HG21 | 37:BC:119:ASP:CG   | 2.18                     | 0.64              |
| 47:BO:104:ARG:HH21 | 52:BT:33:LYS:HE3   | 1.62                     | 0.64              |
| 57:BY:17:SER:HB2   | 57:BY:71:LYS:NZ    | 2.11                     | 0.64              |
| 58:BZ:108:PRO:HB3  | 58:BZ:141:VAL:HG12 | 1.78                     | 0.64              |
| 1:AA:1432:G:OP1    | 52:BT:107:ASP:HB2  | 1.98                     | 0.64              |
| 1:AA:39:G:C8       | 1:AA:498:U:N3      | 2.44                     | 0.64              |
| 1:AA:788:U:H3      | 1:AA:792:A:HO2'    | 1.43                     | 0.64              |
| 11:AK:97:ALA:O     | 11:AK:101:SER:HB3  | 1.97                     | 0.64              |
| 12:AL:27:LEU:CD1   | 12:AL:28:LYS:HG3   | 2.27                     | 0.64              |
| 24:AY:98:MET:CG    | 24:AY:125:ALA:HA   | 2.28                     | 0.64              |
| 35:BA:1036:G:C6    | 35:BA:1120:G:C6    | 2.86                     | 0.64              |
| 35:BA:1984:G:C2'   | 35:BA:1985:G:C5'   | 2.75                     | 0.64              |
| 35:BA:2360:A:HO2'  | 35:BA:2361:A:H5''  | 1.58                     | 0.64              |
| 35:BA:2756:U:C1'   | 35:BA:2757:A:P     | 2.86                     | 0.64              |
| 35:BA:37:C:H2'     | 35:BA:38:A:H8      | 1.63                     | 0.64              |
| 35:BA:49:A:O5'     | 35:BA:51:G:H5'     | 1.97                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:53:A:H2'     | 35:BA:54:G:C5'     | 2.24                     | 0.64              |
| 36:BB:13:A:O2'     | 36:BB:14:U:H3'     | 1.98                     | 0.64              |
| 39:BE:11:MET:HB2   | 39:BE:23:VAL:O     | 1.96                     | 0.64              |
| 41:BG:131:TYR:O    | 41:BG:132:ASN:HB2  | 1.96                     | 0.64              |
| 41:BG:96:ARG:O     | 41:BG:99:MET:HB3   | 1.97                     | 0.64              |
| 50:BR:50:HIS:NE2   | 50:BR:54:LEU:HD11  | 2.13                     | 0.64              |
| 54:BV:65:GLY:HA3   | 54:BV:91:TYR:CZ    | 2.32                     | 0.64              |
| 57:BY:17:SER:OG    | 57:BY:18:GLY:N     | 2.30                     | 0.64              |
| 58:BZ:145:GLU:HG3  | 58:BZ:146:ILE:H    | 1.63                     | 0.64              |
| 3:AC:11:ARG:O      | 3:AC:12:LEU:C      | 2.35                     | 0.64              |
| 3:AC:25:GLY:O      | 3:AC:27:LYS:N      | 2.31                     | 0.64              |
| 12:AL:86:ARG:O     | 12:AL:86:ARG:HG2   | 1.98                     | 0.64              |
| 24:AY:438:PHE:CZ   | 24:AY:451:ILE:HG13 | 2.32                     | 0.64              |
| 24:AY:546:ILE:HD13 | 24:AY:565:VAL:HG11 | 1.79                     | 0.64              |
| 29:B4:33:VAL:CG1   | 29:B4:34:GLU:N     | 2.54                     | 0.64              |
| 35:BA:1797:C:O2'   | 35:BA:1798:U:H5'   | 1.97                     | 0.64              |
| 35:BA:325:G:H2'    | 35:BA:326:G:H8     | 1.63                     | 0.64              |
| 30:B5:16:ARG:NH2   | 35:BA:517:C:OP1    | 2.31                     | 0.64              |
| 36:BB:2:C:H2'      | 36:BB:3:C:H6       | 1.63                     | 0.64              |
| 39:BE:48:GLN:HE21  | 39:BE:78:LEU:HD22  | 1.62                     | 0.64              |
| 50:BR:97:VAL:O     | 50:BR:98:LEU:HD23  | 1.96                     | 0.64              |
| 57:BY:44:ILE:N     | 57:BY:44:ILE:HD12  | 2.12                     | 0.64              |
| 1:AA:1184:G:C2'    | 1:AA:1185:G:H5'    | 2.28                     | 0.64              |
| 1:AA:188:C:C2      | 1:AA:189:G:N7      | 2.66                     | 0.64              |
| 2:AB:87:ARG:NH2    | 2:AB:233:SER:H     | 1.96                     | 0.64              |
| 9:AI:4:TYR:CD2     | 9:AI:88:TYR:HB2    | 2.33                     | 0.64              |
| 26:B1:50:ARG:HA    | 26:B1:59:THR:HA    | 1.80                     | 0.64              |
| 35:BA:1221:C:H2'   | 35:BA:1221(A):C:C6 | 2.32                     | 0.64              |
| 35:BA:2124:G:O2'   | 35:BA:2125:G:H5'   | 1.96                     | 0.64              |
| 35:BA:2555:U:C3'   | 35:BA:2556:C:H5'   | 2.27                     | 0.64              |
| 35:BA:465:G:C6     | 35:BA:466:A:N6     | 2.65                     | 0.64              |
| 35:BA:52:A:O2'     | 35:BA:53:A:H5'     | 1.97                     | 0.64              |
| 35:BA:607:U:O4     | 35:BA:620:G:C4     | 2.51                     | 0.64              |
| 35:BA:699:A:H2'    | 35:BA:700:G:C5'    | 2.28                     | 0.64              |
| 41:BG:104:GLU:HB3  | 41:BG:105:LYS:HE2  | 1.79                     | 0.64              |
| 42:BH:136:ILE:HD12 | 42:BH:136:ILE:N    | 2.13                     | 0.64              |
| 42:BH:98:LEU:HD12  | 42:BH:102:ALA:O    | 1.98                     | 0.64              |
| 46:BN:57:ALA:O     | 46:BN:58:ASP:O     | 2.15                     | 0.64              |
| 49:BQ:52:VAL:O     | 49:BQ:56:ARG:HB2   | 1.97                     | 0.64              |
| 51:BS:66:ALA:HA    | 51:BS:69:VAL:CG1   | 2.26                     | 0.64              |
| 1:AA:58:C:O5'      | 1:AA:58:C:H6       | 1.80                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:710:G:OP1     | 6:AF:54:LYS:HE3    | 1.98                     | 0.64              |
| 3:AC:11:ARG:HH11   | 3:AC:11:ARG:HG2    | 1.63                     | 0.64              |
| 19:AS:49:ILE:O     | 19:AS:60:VAL:HG12  | 1.98                     | 0.64              |
| 24:AY:99:ARG:HG2   | 24:AY:401:SER:OG   | 1.97                     | 0.64              |
| 25:B0:53:MET:HG3   | 25:B0:57:PHE:HA    | 1.79                     | 0.64              |
| 27:B2:2:LYS:HE3    | 27:B2:52:ASP:OD1   | 1.97                     | 0.64              |
| 28:B3:1:MET:HB3    | 28:B3:2:PRO:CD     | 2.22                     | 0.64              |
| 29:B4:22:ILE:HG23  | 41:BG:105:LYS:HD3  | 1.79                     | 0.64              |
| 33:B8:50:LEU:C     | 33:B8:52:LYS:H     | 2.01                     | 0.64              |
| 33:B8:52:LYS:N     | 33:B8:53:PRO:CD    | 2.60                     | 0.64              |
| 35:BA:1701:A:H2'   | 35:BA:1702:G:H5'   | 1.80                     | 0.64              |
| 35:BA:2123:G:N1    | 35:BA:2176:A:C6    | 2.66                     | 0.64              |
| 35:BA:2581:G:C5    | 35:BA:2610:C:N4    | 2.66                     | 0.64              |
| 25:B0:44:ARG:NH2   | 35:BA:858:U:OP1    | 2.29                     | 0.64              |
| 38:BD:123:ALA:HB3  | 38:BD:131:LEU:HG   | 1.80                     | 0.64              |
| 40:BF:89:VAL:HG12  | 40:BF:90:PHE:H     | 1.63                     | 0.64              |
| 41:BG:144:ILE:HG23 | 41:BG:145:THR:N    | 2.12                     | 0.64              |
| 48:BP:81:GLN:NE2   | 48:BP:106:LEU:HA   | 2.12                     | 0.64              |
| 55:BW:69:LEU:HA    | 55:BW:108:GLY:O    | 1.98                     | 0.64              |
| 55:BW:90:ARG:HH11  | 55:BW:90:ARG:HG3   | 1.62                     | 0.64              |
| 57:BY:88:LYS:NZ    | 57:BY:93:GLY:HA3   | 2.13                     | 0.64              |
| 1:AA:263:A:O2'     | 1:AA:264:U:H5'     | 1.98                     | 0.64              |
| 2:AB:17:PHE:CB     | 2:AB:44:LEU:HD11   | 2.24                     | 0.64              |
| 9:AI:47:LEU:C      | 9:AI:49:PRO:HD2    | 2.18                     | 0.64              |
| 10:AJ:90:LEU:H     | 10:AJ:91:PRO:HD2   | 1.61                     | 0.64              |
| 24:AY:17:ILE:CD1   | 24:AY:81:ILE:CG2   | 2.76                     | 0.64              |
| 24:AY:386:GLY:HA3  | 24:AY:402:ILE:HG12 | 1.77                     | 0.64              |
| 24:AY:471:LYS:O    | 24:AY:471:LYS:HG2  | 1.98                     | 0.64              |
| 25:B0:69:PHE:CG    | 25:B0:79:VAL:HG22  | 2.33                     | 0.64              |
| 35:BA:1173:G:H5'   | 35:BA:1174:A:O5'   | 1.98                     | 0.64              |
| 35:BA:1770:G:H2'   | 35:BA:1771:C:C5'   | 2.27                     | 0.64              |
| 35:BA:37:C:H2'     | 35:BA:38:A:C8      | 2.33                     | 0.64              |
| 35:BA:654(O):G:H2' | 35:BA:654(P):C:C5  | 2.33                     | 0.64              |
| 35:BA:1113:U:P     | 42:BH:1:MET:H1     | 2.21                     | 0.64              |
| 48:BP:9:ASN:H      | 48:BP:10:PRO:CD    | 2.11                     | 0.64              |
| 48:BP:65:ARG:CB    | 48:BP:68:GLN:HE22  | 2.06                     | 0.64              |
| 51:BS:24:LEU:HB3   | 51:BS:85:VAL:HG12  | 1.78                     | 0.64              |
| 53:BU:95:LEU:C     | 53:BU:97:ASP:H     | 2.02                     | 0.64              |
| 1:AA:1241:G:H2'    | 1:AA:1242:C:C6     | 2.33                     | 0.64              |
| 24:AY:31:ARG:HH11  | 24:AY:31:ARG:HA    | 1.61                     | 0.64              |
| 29:B4:16:CYS:HA    | 29:B4:33:VAL:CG2   | 2.26                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:B4:56:VAL:HG22  | 29:B4:57:GLU:N    | 2.11                     | 0.64              |
| 35:BA:1449:A:H5'   | 35:BA:1450:G:OP2  | 1.97                     | 0.64              |
| 35:BA:1808:U:C2'   | 35:BA:1809:A:H5'  | 2.28                     | 0.64              |
| 35:BA:1847:A:H4'   | 35:BA:1848:A:OP2  | 1.97                     | 0.64              |
| 35:BA:2361:A:C2'   | 35:BA:2362:G:H5'  | 2.28                     | 0.64              |
| 35:BA:247:G:OP2    | 35:BA:249:C:N4    | 2.30                     | 0.64              |
| 35:BA:2567:G:H2'   | 35:BA:2568:C:C6   | 2.32                     | 0.64              |
| 35:BA:696:G:C2'    | 35:BA:697:C:H5'   | 2.28                     | 0.64              |
| 38:BD:30:GLU:HG3   | 38:BD:63:ARG:NH2  | 2.12                     | 0.64              |
| 40:BF:165:ARG:HH11 | 40:BF:165:ARG:HB3 | 1.64                     | 0.64              |
| 40:BF:3:GLU:HA     | 40:BF:24:LEU:CB   | 2.28                     | 0.64              |
| 47:BO:65:THR:HA    | 47:BO:82:ASN:HD22 | 1.63                     | 0.64              |
| 54:BV:19:LYS:CE    | 54:BV:20:LEU:H    | 2.11                     | 0.64              |
| 1:AA:1077:G:N1     | 1:AA:1081:G:O6    | 2.30                     | 0.63              |
| 1:AA:1199:U:H4'    | 10:AJ:54:PHE:CE1  | 2.33                     | 0.63              |
| 1:AA:163:C:H2'     | 1:AA:164:U:C6     | 2.33                     | 0.63              |
| 1:AA:361:G:O2'     | 1:AA:362:G:H5'    | 1.98                     | 0.63              |
| 1:AA:60:A:O2'      | 1:AA:61:G:P       | 2.56                     | 0.63              |
| 12:AL:60:LEU:HD21  | 12:AL:66:VAL:HG22 | 1.80                     | 0.63              |
| 10:AJ:65:LEU:HD13  | 14:AN:56:VAL:HG23 | 1.80                     | 0.63              |
| 29:B4:34:GLU:O     | 29:B4:35:VAL:C    | 2.36                     | 0.63              |
| 34:B9:10:ILE:CD1   | 34:B9:34:GLN:HE22 | 2.10                     | 0.63              |
| 35:BA:2581:G:N9    | 35:BA:2610:C:N4   | 2.46                     | 0.63              |
| 35:BA:2681:C:H5    | 35:BA:2725:A:N6   | 1.93                     | 0.63              |
| 35:BA:2756:U:C4    | 35:BA:2759:G:O6   | 2.51                     | 0.63              |
| 35:BA:331:A:H1'    | 35:BA:332:A:OP1   | 1.96                     | 0.63              |
| 35:BA:389:G:N1     | 48:BP:70:GLN:HG3  | 2.13                     | 0.63              |
| 37:BC:121:MET:HA   | 37:BC:124:VAL:CG1 | 2.27                     | 0.63              |
| 38:BD:108:PRO:HB3  | 38:BD:143:HIS:CE1 | 2.33                     | 0.63              |
| 41:BG:106:LEU:O    | 41:BG:110:ALA:HB3 | 1.97                     | 0.63              |
| 41:BG:48:GLU:CD    | 41:BG:49:ASP:H    | 2.00                     | 0.63              |
| 41:BG:93:THR:HG22  | 41:BG:94:LEU:N    | 2.12                     | 0.63              |
| 54:BV:38:LEU:C     | 54:BV:39:LEU:HD13 | 2.18                     | 0.63              |
| 13:AM:11:ARG:C     | 13:AM:13:LYS:H    | 2.01                     | 0.63              |
| 24:AY:431:LEU:HD11 | 24:AY:465:ARG:NH1 | 2.12                     | 0.63              |
| 34:B9:36:GLN:HG2   | 35:BA:1124:C:O2'  | 1.99                     | 0.63              |
| 35:BA:1170:G:H1    | 35:BA:1179:C:N4   | 1.94                     | 0.63              |
| 32:B7:32:LYS:NZ    | 35:BA:181:A:OP1   | 2.32                     | 0.63              |
| 35:BA:2036:C:C2'   | 35:BA:2037:G:H5'  | 2.29                     | 0.63              |
| 35:BA:2189:U:H2'   | 35:BA:2190:G:C5'  | 2.17                     | 0.63              |
| 35:BA:605:C:O2'    | 35:BA:606:U:C5'   | 2.33                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:627:A:C4'    | 35:BA:628:G:OP1    | 2.31                     | 0.63              |
| 37:BC:68:GLY:N     | 37:BC:189:ASN:HD21 | 1.96                     | 0.63              |
| 38:BD:35:LYS:HZ2   | 38:BD:36:PRO:N     | 1.96                     | 0.63              |
| 41:BG:66:GLN:HE22  | 41:BG:94:LEU:CG    | 2.11                     | 0.63              |
| 54:BV:39:LEU:CD1   | 54:BV:47:VAL:HG11  | 2.27                     | 0.63              |
| 58:BZ:71:VAL:HG11  | 58:BZ:74:VAL:HG23  | 1.78                     | 0.63              |
| 1:AA:539:A:H2'     | 1:AA:540:G:H8      | 1.64                     | 0.63              |
| 1:AA:592:G:C2      | 1:AA:593:G:C8      | 2.86                     | 0.63              |
| 3:AC:15:THR:HG23   | 3:AC:181:ASN:HA    | 1.80                     | 0.63              |
| 3:AC:71:ALA:HB2    | 3:AC:115:LEU:HD21  | 1.78                     | 0.63              |
| 3:AC:84:ILE:O      | 3:AC:86:VAL:N      | 2.31                     | 0.63              |
| 19:AS:7:LYS:O      | 19:AS:7:LYS:HG2    | 1.98                     | 0.63              |
| 1:AA:190:U:N3      | 20:AT:105:SER:HB2  | 2.13                     | 0.63              |
| 24:AY:17:ILE:HD13  | 24:AY:81:ILE:CG2   | 2.29                     | 0.63              |
| 33:B8:13:ARG:HD2   | 48:BP:61:ARG:CD    | 2.20                     | 0.63              |
| 35:BA:1282:U:C2    | 35:BA:1286:A:N6    | 2.66                     | 0.63              |
| 35:BA:2363:C:H2'   | 35:BA:2364:C:C6    | 2.33                     | 0.63              |
| 35:BA:654(T):C:O2' | 35:BA:654(U):A:O4' | 2.16                     | 0.63              |
| 35:BA:967:C:O2'    | 35:BA:968:G:H5''   | 1.97                     | 0.63              |
| 39:BE:132:HIS:ND1  | 39:BE:132:HIS:O    | 2.30                     | 0.63              |
| 35:BA:1022:G:O6    | 46:BN:66:LYS:HE3   | 1.99                     | 0.63              |
| 48:BP:136:GLU:O    | 48:BP:139:LYS:HB2  | 1.98                     | 0.63              |
| 51:BS:61:ASN:HB3   | 51:BS:64:GLU:HB2   | 1.78                     | 0.63              |
| 54:BV:12:TYR:CD1   | 54:BV:12:TYR:N     | 2.66                     | 0.63              |
| 35:BA:310:A:OP1    | 57:BY:17:SER:O     | 2.16                     | 0.63              |
| 58:BZ:30:ASN:O     | 58:BZ:32:HIS:N     | 2.31                     | 0.63              |
| 1:AA:1158:C:O2     | 1:AA:1158:C:C2'    | 2.47                     | 0.63              |
| 1:AA:60:A:O2'      | 1:AA:61:G:H5''     | 1.98                     | 0.63              |
| 2:AB:19:HIS:CE1    | 2:AB:206:ASP:HB2   | 2.33                     | 0.63              |
| 10:AJ:78:ASN:ND2   | 10:AJ:80:LYS:HB2   | 2.14                     | 0.63              |
| 12:AL:123:LYS:CE   | 12:AL:123:LYS:H    | 2.11                     | 0.63              |
| 26:B1:52:ARG:NH1   | 35:BA:2218:U:O2'   | 2.32                     | 0.63              |
| 35:BA:2757:A:O2'   | 35:BA:2758:A:H5''  | 1.98                     | 0.63              |
| 35:BA:463:G:N2     | 35:BA:466:A:OP2    | 2.30                     | 0.63              |
| 35:BA:694:U:H6     | 35:BA:694:U:O5'    | 1.80                     | 0.63              |
| 35:BA:702:G:O2'    | 35:BA:703:U:C5'    | 2.30                     | 0.63              |
| 37:BC:101:ILE:C    | 37:BC:103:LYS:H    | 1.99                     | 0.63              |
| 47:BO:104:ARG:HH21 | 52:BT:33:LYS:CE    | 2.12                     | 0.63              |
| 1:AA:942:G:N3      | 1:AA:943:U:C6      | 2.67                     | 0.63              |
| 1:AA:973:G:H3'     | 1:AA:974:A:H5''    | 1.81                     | 0.63              |
| 9:AI:28:VAL:O      | 9:AI:29:ASN:HB2    | 1.99                     | 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    | 2.12                     | 0.63              |
| 24:AY:84:THR:CG2  | 24:AY:94:VAL:HG22  | 2.27                     | 0.63              |
| 35:BA:1301:A:O2'  | 35:BA:1302:A:P     | 2.55                     | 0.63              |
| 35:BA:1434:A:H61  | 35:BA:1558:A:N6    | 1.95                     | 0.63              |
| 35:BA:1805:U:HO2' | 35:BA:1806:C:H5'   | 1.61                     | 0.63              |
| 35:BA:327:G:C2'   | 35:BA:328:U:O5'    | 2.47                     | 0.63              |
| 37:BC:115:VAL:HA  | 37:BC:139:PRO:HB3  | 1.80                     | 0.63              |
| 38:BD:186:HIS:CD2 | 38:BD:188:GLU:H    | 2.16                     | 0.63              |
| 48:BP:51:PHE:CA   | 48:BP:52:GLU:CB    | 2.70                     | 0.63              |
| 56:BX:53:LYS:HB3  | 56:BX:82:GLN:HB3   | 1.79                     | 0.63              |
| 1:AA:1116:C:H2'   | 1:AA:1117:G:C5'    | 2.29                     | 0.63              |
| 1:AA:1195:C:H5''  | 1:AA:1196:U:O5'    | 1.99                     | 0.63              |
| 3:AC:180:ALA:O    | 3:AC:181:ASN:HB3   | 1.99                     | 0.63              |
| 3:AC:22:TRP:CZ3   | 3:AC:24:ALA:HB2    | 2.33                     | 0.63              |
| 16:AP:45:THR:HG22 | 16:AP:47:ASP:N     | 2.14                     | 0.63              |
| 25:B0:20:ARG:NH1  | 35:BA:2357:U:OP1   | 2.32                     | 0.63              |
| 33:B8:33:ASN:CG   | 33:B8:34:TRP:H     | 2.01                     | 0.63              |
| 35:BA:1223:G:N2   | 35:BA:1226:A:OP2   | 2.31                     | 0.63              |
| 35:BA:1543:C:H3'  | 35:BA:1544:A:C5'   | 2.28                     | 0.63              |
| 35:BA:1698:A:H4'  | 35:BA:1699:G:OP1   | 1.97                     | 0.63              |
| 35:BA:1925:C:H5'  | 35:BA:1926:U:OP2   | 1.98                     | 0.63              |
| 35:BA:2313:C:C4'  | 41:BG:40:ASN:ND2   | 2.60                     | 0.63              |
| 35:BA:2606:C:O2'  | 35:BA:2607:G:C5'   | 2.46                     | 0.63              |
| 35:BA:28:A:C2'    | 35:BA:29:U:H5'     | 2.28                     | 0.63              |
| 35:BA:860:U:H5    | 35:BA:917:A:N7     | 1.96                     | 0.63              |
| 41:BG:33:ARG:HA   | 41:BG:172:LEU:HD11 | 1.81                     | 0.63              |
| 41:BG:38:VAL:HG13 | 41:BG:93:THR:HA    | 1.81                     | 0.63              |
| 48:BP:78:PRO:HA   | 48:BP:110:TYR:HE2  | 1.64                     | 0.63              |
| 58:BZ:108:PRO:HG2 | 58:BZ:111:VAL:HG23 | 1.80                     | 0.63              |
| 1:AA:314:C:O5'    | 1:AA:314:C:H6      | 1.82                     | 0.63              |
| 1:AA:56:U:H2'     | 1:AA:57:G:C8       | 2.33                     | 0.63              |
| 1:AA:961:U:H1'    | 1:AA:962:C:C5'     | 2.28                     | 0.63              |
| 2:AB:25:ASN:O     | 2:AB:26:PRO:C      | 2.36                     | 0.63              |
| 5:AE:147:ASP:HB3  | 5:AE:150:ARG:NH1   | 2.14                     | 0.63              |
| 7:AG:121:ALA:H    | 7:AG:124:LEU:CD1   | 1.99                     | 0.63              |
| 9:AI:126:SER:O    | 9:AI:127:LYS:HB3   | 1.96                     | 0.63              |
| 10:AJ:22:LYS:HD2  | 10:AJ:90:LEU:HD22  | 1.80                     | 0.63              |
| 35:BA:1086:A:O2'  | 35:BA:1103:A:N6    | 2.31                     | 0.63              |
| 35:BA:1461:G:H2'  | 35:BA:1462:C:H5'   | 1.81                     | 0.63              |
| 35:BA:2423:U:H5'  | 35:BA:2423:U:H6    | 1.63                     | 0.63              |
| 35:BA:848:G:H2'   | 35:BA:849:A:C8     | 2.34                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BC:158:LYS:O    | 37:BC:159:ALA:HB3  | 1.99                     | 0.63              |
| 37:BC:44:VAL:CG2   | 37:BC:176:VAL:HG21 | 2.28                     | 0.63              |
| 39:BE:48:GLN:HE22  | 39:BE:64:LYS:HE3   | 1.62                     | 0.63              |
| 41:BG:65:GLY:O     | 41:BG:66:GLN:CB    | 2.46                     | 0.63              |
| 57:BY:28:LYS:HB2   | 57:BY:38:ILE:N     | 2.10                     | 0.63              |
| 58:BZ:79:ARG:HG3   | 58:BZ:80:ARG:HG2   | 1.81                     | 0.63              |
| 1:AA:105:G:C5      | 1:AA:106:C:N4      | 2.67                     | 0.63              |
| 1:AA:1321:C:C3'    | 1:AA:1322:C:H5''   | 2.29                     | 0.63              |
| 1:AA:491:G:O2'     | 1:AA:492:G:H5'     | 1.98                     | 0.63              |
| 1:AA:942:G:H2'     | 1:AA:943:U:H6      | 1.63                     | 0.63              |
| 3:AC:83:ARG:O      | 3:AC:84:ILE:C      | 2.37                     | 0.63              |
| 13:AM:108:ARG:N    | 13:AM:108:ARG:HD2  | 2.14                     | 0.63              |
| 24:AY:96:ARG:HD3   | 24:AY:314:PHE:O    | 1.99                     | 0.63              |
| 24:AY:56:GLU:O     | 24:AY:57:GLN:C     | 2.37                     | 0.63              |
| 24:AY:614:GLU:HG3  | 24:AY:617:MET:HE3  | 1.80                     | 0.63              |
| 25:B0:66:VAL:HG12  | 25:B0:67:VAL:N     | 2.13                     | 0.63              |
| 26:B1:34:THR:HG22  | 26:B1:36:GLY:H     | 1.63                     | 0.63              |
| 29:B4:16:CYS:SG    | 29:B4:21:VAL:HG23  | 2.37                     | 0.63              |
| 29:B4:7:PRO:HG2    | 29:B4:9:LEU:HD11   | 1.80                     | 0.63              |
| 35:BA:1839:G:H5'   | 35:BA:1839:G:H8    | 1.64                     | 0.63              |
| 35:BA:1890:A:C3'   | 35:BA:1891:G:C5'   | 2.77                     | 0.63              |
| 35:BA:2492:U:O2'   | 35:BA:2493:U:H5'   | 1.99                     | 0.63              |
| 35:BA:848:G:H5'    | 35:BA:848:G:H8     | 1.63                     | 0.63              |
| 37:BC:7:ARG:O      | 37:BC:11:LEU:HD23  | 1.99                     | 0.63              |
| 38:BD:142:VAL:HG23 | 38:BD:192:THR:C    | 2.19                     | 0.63              |
| 38:BD:35:LYS:HB3   | 38:BD:35:LYS:HZ2   | 1.64                     | 0.63              |
| 35:BA:1695:G:H1'   | 38:BD:8:PRO:O      | 1.98                     | 0.63              |
| 41:BG:144:ILE:HG23 | 41:BG:145:THR:H    | 1.62                     | 0.63              |
| 42:BH:22:GLY:O     | 42:BH:37:VAL:N     | 2.27                     | 0.63              |
| 54:BV:5:VAL:HG23   | 54:BV:37:VAL:O     | 1.98                     | 0.63              |
| 1:AA:1049:U:C1'    | 1:AA:1050:G:OP2    | 2.46                     | 0.63              |
| 1:AA:1281:U:C5'    | 1:AA:1282:C:C5     | 2.77                     | 0.63              |
| 1:AA:1286:A:O2'    | 1:AA:1287:A:H4'    | 1.99                     | 0.63              |
| 1:AA:1320:C:H5'    | 1:AA:1320:C:H6     | 1.64                     | 0.63              |
| 1:AA:1348:U:C5     | 1:AA:1373:G:N2     | 2.67                     | 0.63              |
| 1:AA:313:A:H2'     | 1:AA:314:C:C6      | 2.34                     | 0.63              |
| 1:AA:349:A:HO2'    | 1:AA:350:G:H5'     | 1.62                     | 0.63              |
| 2:AB:10:LEU:C      | 2:AB:10:LEU:HD23   | 2.19                     | 0.63              |
| 3:AC:55:VAL:O      | 3:AC:55:VAL:HG12   | 1.97                     | 0.63              |
| 32:B7:8:ASN:ND2    | 32:B7:11:LYS:H     | 1.97                     | 0.63              |
| 35:BA:1646:C:H5''  | 35:BA:1647:G:O5'   | 1.99                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2126:A:H1'   | 35:BA:2127:G:C1'   | 2.29                     | 0.63              |
| 35:BA:89:G:OP2     | 35:BA:90:U:H2'     | 1.99                     | 0.63              |
| 36:BB:28:C:H42     | 36:BB:56:G:H1      | 1.45                     | 0.63              |
| 37:BC:133:GLY:O    | 37:BC:135:ARG:N    | 2.32                     | 0.63              |
| 37:BC:6:LYS:HG3    | 37:BC:7:ARG:N      | 2.14                     | 0.63              |
| 48:BP:55:ARG:HG2   | 48:BP:56:SER:N     | 2.14                     | 0.63              |
| 48:BP:6:LEU:HD12   | 48:BP:9:ASN:OD1    | 1.99                     | 0.63              |
| 50:BR:50:HIS:O     | 50:BR:54:LEU:HD12  | 1.99                     | 0.63              |
| 57:BY:27:VAL:HB    | 57:BY:29:GLU:OE1   | 1.98                     | 0.63              |
| 1:AA:1287:A:C6     | 1:AA:1288:A:C6     | 2.86                     | 0.62              |
| 1:AA:166:G:H2'     | 1:AA:167:G:C8      | 2.34                     | 0.62              |
| 1:AA:198:G:C2      | 1:AA:199:G:C5      | 2.88                     | 0.62              |
| 1:AA:521:G:C2'     | 1:AA:522:C:C5'     | 2.72                     | 0.62              |
| 1:AA:936:C:C2'     | 1:AA:937:A:C5'     | 2.76                     | 0.62              |
| 13:AM:3:ARG:CZ     | 13:AM:7:VAL:HG13   | 2.29                     | 0.62              |
| 19:AS:42:PRO:HB3   | 19:AS:67:VAL:CG1   | 2.29                     | 0.62              |
| 20:AT:71:THR:HG22  | 20:AT:72:LEU:N     | 2.13                     | 0.62              |
| 25:B0:57:PHE:CD1   | 25:B0:57:PHE:N     | 2.67                     | 0.62              |
| 35:BA:2029:G:N1    | 35:BA:2033:A:P     | 2.71                     | 0.62              |
| 35:BA:2445:G:OP1   | 40:BF:74:ARG:NH2   | 2.32                     | 0.62              |
| 35:BA:247:G:H4'    | 35:BA:386:G:C5     | 2.34                     | 0.62              |
| 35:BA:408:G:O2'    | 35:BA:409:C:H5'    | 1.99                     | 0.62              |
| 35:BA:968:G:H2'    | 35:BA:969:U:H6     | 1.64                     | 0.62              |
| 39:BE:68:ALA:C     | 39:BE:70:ALA:H     | 2.02                     | 0.62              |
| 40:BF:51:THR:HB    | 40:BF:88:VAL:HG11  | 1.80                     | 0.62              |
| 41:BG:129:GLY:HA3  | 41:BG:169:ALA:HB2  | 1.81                     | 0.62              |
| 53:BU:95:LEU:HD13  | 54:BV:4:ILE:HG23   | 1.80                     | 0.62              |
| 58:BZ:18:LEU:O     | 58:BZ:21:ALA:HB3   | 1.99                     | 0.62              |
| 1:AA:61:G:C6       | 1:AA:107:G:C6      | 2.88                     | 0.62              |
| 1:AA:1305:G:H5'    | 21:AU:4:GLY:CA     | 2.28                     | 0.62              |
| 1:AA:200:G:H1      | 1:AA:217:C:H42     | 1.46                     | 0.62              |
| 1:AA:788:U:H2'     | 1:AA:789:U:H5'     | 1.80                     | 0.62              |
| 2:AB:204:ASN:HD22  | 2:AB:205:ASP:H     | 1.44                     | 0.62              |
| 2:AB:82:ARG:HG3    | 2:AB:82:ARG:NH1    | 2.13                     | 0.62              |
| 24:AY:262:SER:OG   | 24:AY:265:LYS:HB2  | 1.98                     | 0.62              |
| 28:B3:7:LYS:CG     | 28:B3:32:GLN:O     | 2.45                     | 0.62              |
| 28:B3:4:LEU:HD11   | 28:B3:44:ARG:CZ    | 2.29                     | 0.62              |
| 26:B1:3:LYS:NZ     | 35:BA:1364:G:C8    | 2.65                     | 0.62              |
| 35:BA:146:G:H5'    | 35:BA:146:G:C8     | 2.32                     | 0.62              |
| 35:BA:2134:A:H5'   | 35:BA:2134:A:H8    | 1.64                     | 0.62              |
| 35:BA:363(E):U:H5' | 35:BA:363(F):A:OP2 | 1.98                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BB:34:U:O4     | 36:BB:44:G:H2'     | 1.99                     | 0.62              |
| 37:BC:29:LEU:O    | 37:BC:32:GLU:N     | 2.31                     | 0.62              |
| 38:BD:24:ILE:CD1  | 38:BD:25:THR:N     | 2.61                     | 0.62              |
| 41:BG:85:GLY:O    | 41:BG:86:MET:HB2   | 1.99                     | 0.62              |
| 42:BH:18:GLU:HG3  | 42:BH:25:LYS:HB2   | 1.81                     | 0.62              |
| 52:BT:102:ILE:O   | 52:BT:106:SER:HB3  | 1.99                     | 0.62              |
| 47:BO:104:ARG:HE  | 52:BT:33:LYS:HE3   | 1.63                     | 0.62              |
| 52:BT:98:LYS:HB3  | 52:BT:100:TYR:CE2  | 2.34                     | 0.62              |
| 1:AA:192:U:C1'    | 20:AT:103:GLY:HA2  | 2.28                     | 0.62              |
| 1:AA:346:G:H5''   | 52:BT:35:LYS:HZ1   | 1.65                     | 0.62              |
| 1:AA:560:U:H5'    | 1:AA:561:U:H3'     | 1.80                     | 0.62              |
| 4:AD:17:VAL:CG1   | 4:AD:18:LYS:N      | 2.54                     | 0.62              |
| 9:AI:52:ALA:HB3   | 9:AI:95:LYS:NZ     | 2.13                     | 0.62              |
| 1:AA:963:G:H21    | 10:AJ:55:LYS:CE    | 2.11                     | 0.62              |
| 14:AN:13:THR:N    | 14:AN:14:PRO:CD    | 2.61                     | 0.62              |
| 24:AY:25:LYS:NZ   | 24:AY:86:GLY:CA    | 2.62                     | 0.62              |
| 25:B0:36:ILE:CG1  | 25:B0:36:ILE:O     | 2.41                     | 0.62              |
| 31:B6:11:LEU:HD22 | 31:B6:11:LEU:C     | 2.19                     | 0.62              |
| 35:BA:2130:U:O3'  | 35:BA:2133:A:H5'   | 2.00                     | 0.62              |
| 35:BA:2822:G:O6   | 50:BR:4:LEU:HD22   | 2.00                     | 0.62              |
| 35:BA:752:A:O2'   | 35:BA:753:C:OP2    | 2.16                     | 0.62              |
| 37:BC:73:VAL:HG13 | 37:BC:74:ARG:N     | 2.15                     | 0.62              |
| 40:BF:3:GLU:HA    | 40:BF:24:LEU:HB3   | 1.80                     | 0.62              |
| 51:BS:106:ARG:CB  | 51:BS:106:ARG:HH11 | 2.05                     | 0.62              |
| 1:AA:1042:G:O2'   | 1:AA:1043:C:H5'    | 2.00                     | 0.62              |
| 1:AA:1076:C:C2'   | 1:AA:1077:G:H5'    | 2.29                     | 0.62              |
| 1:AA:495:A:C1'    | 1:AA:496:A:H2'     | 2.28                     | 0.62              |
| 1:AA:559:A:H4'    | 1:AA:560:U:H5''    | 1.80                     | 0.62              |
| 1:AA:863:U:C5'    | 1:AA:863:U:O2      | 2.47                     | 0.62              |
| 3:AC:131:ARG:HB2  | 3:AC:131:ARG:HH11  | 1.65                     | 0.62              |
| 22:AV:12:U:H3     | 22:AV:23:A:N6      | 1.97                     | 0.62              |
| 25:B0:45:PHE:HZ   | 25:B0:77:ARG:HH21  | 1.47                     | 0.62              |
| 28:B3:8:LEU:HD23  | 28:B3:53:LEU:O     | 2.00                     | 0.62              |
| 35:BA:1107:G:H4'  | 43:BJ:81:UNK:HA    | 1.80                     | 0.62              |
| 35:BA:2137:C:H2'  | 35:BA:2138:C:C6    | 2.35                     | 0.62              |
| 35:BA:48:G:O3'    | 35:BA:51:G:H5'     | 1.99                     | 0.62              |
| 35:BA:518:G:H4'   | 55:BW:18:ARG:NH1   | 2.15                     | 0.62              |
| 35:BA:774:A:H2    | 35:BA:787:U:O2'    | 1.81                     | 0.62              |
| 38:BD:35:LYS:C    | 38:BD:35:LYS:HD2   | 2.19                     | 0.62              |
| 35:BA:2580:U:C5'  | 39:BE:131:ALA:HB2  | 2.29                     | 0.62              |
| 42:BH:70:THR:HG22 | 42:BH:74:ASN:ND2   | 2.13                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BN:25:ARG:HH11  | 46:BN:25:ARG:HG3   | 1.65                     | 0.62              |
| 52:BT:27:THR:O     | 52:BT:28:VAL:HG12  | 2.00                     | 0.62              |
| 54:BV:49:THR:HB    | 54:BV:50:PRO:CD    | 2.28                     | 0.62              |
| 57:BY:39:VAL:O     | 57:BY:40:GLU:HG2   | 1.99                     | 0.62              |
| 1:AA:505:G:H2'     | 1:AA:506:G:H8      | 1.65                     | 0.62              |
| 1:AA:946:A:H2'     | 1:AA:947:G:H8      | 1.61                     | 0.62              |
| 2:AB:129:GLU:O     | 2:AB:130:ARG:C     | 2.38                     | 0.62              |
| 2:AB:73:THR:HA     | 2:AB:94:ASN:O      | 2.00                     | 0.62              |
| 1:AA:564:C:O2'     | 8:AH:91:ARG:NH2    | 2.33                     | 0.62              |
| 24:AY:590:ILE:HG22 | 24:AY:594:VAL:HG23 | 1.82                     | 0.62              |
| 35:BA:1093:G:H1'   | 35:BA:1099:G:H22   | 1.65                     | 0.62              |
| 35:BA:1902:C:C5'   | 38:BD:246:PRO:HD3  | 2.30                     | 0.62              |
| 35:BA:1925:C:H3'   | 35:BA:1926:U:C5'   | 2.29                     | 0.62              |
| 35:BA:2123:G:O6    | 35:BA:2176:A:N6    | 2.31                     | 0.62              |
| 35:BA:2185:C:HO2'  | 35:BA:2186:G:H8    | 1.48                     | 0.62              |
| 40:BF:185:ASP:HA   | 40:BF:188:ARG:CG   | 2.30                     | 0.62              |
| 41:BG:104:GLU:C    | 41:BG:105:LYS:HE2  | 2.20                     | 0.62              |
| 46:BN:96:GLU:H     | 46:BN:96:GLU:CD    | 2.00                     | 0.62              |
| 47:BO:13:ASN:H     | 47:BO:13:ASN:HD22  | 1.46                     | 0.62              |
| 47:BO:66:LYS:H     | 47:BO:82:ASN:HD21  | 1.47                     | 0.62              |
| 55:BW:36:LEU:HD22  | 55:BW:36:LEU:N     | 2.15                     | 0.62              |
| 56:BX:87:GLN:O     | 56:BX:88:LYS:HD3   | 1.98                     | 0.62              |
| 57:BY:17:SER:HB2   | 57:BY:71:LYS:CE    | 2.29                     | 0.62              |
| 58:BZ:165:VAL:CG1  | 58:BZ:166:SER:N    | 2.61                     | 0.62              |
| 1:AA:1510:U:H2'    | 1:AA:1511:G:C8     | 2.34                     | 0.62              |
| 1:AA:274:A:O2'     | 1:AA:275:G:H8      | 1.83                     | 0.62              |
| 3:AC:130:VAL:HG13  | 3:AC:157:ILE:CG2   | 2.29                     | 0.62              |
| 15:AO:53:HIS:O     | 15:AO:56:LEU:HB3   | 2.00                     | 0.62              |
| 35:BA:1786:A:N9    | 35:BA:1938:A:N6    | 2.47                     | 0.62              |
| 35:BA:1906:G:H3'   | 35:BA:1907:G:H5''  | 1.80                     | 0.62              |
| 35:BA:2581:G:C4    | 35:BA:2610:C:C4    | 2.88                     | 0.62              |
| 38:BD:276:LYS:HD3  | 38:BD:276:LYS:OXT  | 1.99                     | 0.62              |
| 39:BE:47:VAL:HG23  | 39:BE:84:PHE:HB3   | 1.81                     | 0.62              |
| 40:BF:135:LYS:H    | 40:BF:166:ALA:HB2  | 1.64                     | 0.62              |
| 40:BF:54:ARG:CZ    | 40:BF:80:ALA:HB2   | 2.29                     | 0.62              |
| 41:BG:142:PRO:O    | 41:BG:143:GLU:C    | 2.37                     | 0.62              |
| 55:BW:20:VAL:CG2   | 55:BW:47:VAL:HG21  | 2.29                     | 0.62              |
| 1:AA:1160:G:C6     | 1:AA:1181:G:O6     | 2.52                     | 0.62              |
| 1:AA:312:C:O2'     | 1:AA:313:A:C5'     | 2.46                     | 0.62              |
| 1:AA:942:G:N2      | 1:AA:943:U:C2      | 2.67                     | 0.62              |
| 3:AC:25:GLY:C      | 3:AC:27:LYS:H      | 2.03                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:AD:110:PHE:CD1   | 4:AD:110:PHE:N    | 2.56                     | 0.62              |
| 1:AA:963:G:H21     | 10:AJ:55:LYS:HD3  | 1.64                     | 0.62              |
| 13:AM:53:VAL:CG1   | 13:AM:57:ARG:HH21 | 2.13                     | 0.62              |
| 24:AY:252:ASP:HB3  | 24:AY:254:LYS:HZ1 | 1.65                     | 0.62              |
| 24:AY:100:VAL:HG21 | 24:AY:314:PHE:CE1 | 2.35                     | 0.62              |
| 27:B2:5:GLU:CA     | 27:B2:8:LYS:HD2   | 2.27                     | 0.62              |
| 35:BA:2887:U:H2'   | 35:BA:2888:C:C6   | 2.34                     | 0.62              |
| 38:BD:4:LYS:HB3    | 38:BD:18:VAL:HG13 | 1.82                     | 0.62              |
| 40:BF:10:PRO:HA    | 40:BF:127:GLU:HB3 | 1.82                     | 0.62              |
| 39:BE:111:ARG:CA   | 50:BR:2:ARG:HG2   | 2.30                     | 0.62              |
| 52:BT:106:SER:HA   | 52:BT:110:ILE:CG1 | 2.29                     | 0.62              |
| 53:BU:49:HIS:C     | 53:BU:51:LYS:H    | 2.03                     | 0.62              |
| 1:AA:1077:G:N2     | 1:AA:1080:A:OP2   | 2.30                     | 0.62              |
| 1:AA:1152:A:C6     | 1:AA:1153:C:N4    | 2.68                     | 0.62              |
| 1:AA:405:U:H3'     | 1:AA:406:G:H5'    | 1.82                     | 0.62              |
| 1:AA:92:C:H2'      | 1:AA:93:G:H5'     | 1.82                     | 0.62              |
| 1:AA:963:G:H21     | 10:AJ:55:LYS:CD   | 2.13                     | 0.62              |
| 2:AB:25:ASN:O      | 2:AB:27:LYS:N     | 2.33                     | 0.62              |
| 12:AL:46:LYS:O     | 12:AL:48:PRO:HD2  | 1.99                     | 0.62              |
| 13:AM:66:LEU:HD12  | 13:AM:66:LEU:N    | 2.14                     | 0.62              |
| 17:AQ:65:ILE:N     | 17:AQ:65:ILE:HD12 | 2.14                     | 0.62              |
| 22:AV:41:C:O2'     | 22:AV:42:C:C5'    | 2.32                     | 0.62              |
| 24:AY:459:LEU:HD12 | 24:AY:459:LEU:H   | 1.65                     | 0.62              |
| 25:B0:12:ASN:HA    | 25:B0:14:ARG:HH12 | 1.64                     | 0.62              |
| 25:B0:56:ASP:O     | 25:B0:58:THR:N    | 2.33                     | 0.62              |
| 35:BA:1019:U:O2'   | 35:BA:1021:A:H2   | 1.82                     | 0.62              |
| 35:BA:1806:C:HO2'  | 35:BA:1807:G:H5'  | 1.62                     | 0.62              |
| 35:BA:1932:A:H2'   | 35:BA:1933:G:O4'  | 1.99                     | 0.62              |
| 35:BA:2305:A:C2    | 35:BA:2306:C:H1'  | 2.35                     | 0.62              |
| 35:BA:247:G:O2'    | 35:BA:248:G:C5'   | 2.47                     | 0.62              |
| 35:BA:41:C:H42     | 35:BA:437:G:H1    | 1.47                     | 0.62              |
| 35:BA:965:C:C2'    | 35:BA:966:G:H5'   | 2.30                     | 0.62              |
| 37:BC:11:LEU:HD12  | 37:BC:33:LEU:HA   | 1.82                     | 0.62              |
| 42:BH:89:ILE:CD1   | 42:BH:94:TYR:HB3  | 2.29                     | 0.62              |
| 46:BN:58:ASP:O     | 46:BN:59:LYS:C    | 2.38                     | 0.62              |
| 35:BA:389:G:N1     | 48:BP:71:VAL:HG12 | 2.15                     | 0.62              |
| 56:BX:8:ILE:N      | 56:BX:8:ILE:HD12  | 2.15                     | 0.62              |
| 58:BZ:17:ALA:HA    | 58:BZ:20:ARG:CG   | 2.30                     | 0.62              |
| 1:AA:359:U:O2'     | 1:AA:360:A:C5'    | 2.30                     | 0.62              |
| 1:AA:436:C:H2'     | 1:AA:437:U:C6     | 2.35                     | 0.62              |
| 1:AA:556:C:H2'     | 1:AA:557:G:C5'    | 2.27                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:688:G:O6      | 1:AA:700:G:O6      | 2.17                     | 0.62              |
| 1:AA:936:C:H2'     | 1:AA:937:A:C8      | 2.32                     | 0.62              |
| 2:AB:87:ARG:O      | 2:AB:87:ARG:HG2    | 1.99                     | 0.62              |
| 2:AB:91:PRO:O      | 2:AB:92:TYR:HB3    | 2.00                     | 0.62              |
| 3:AC:50:ALA:HB2    | 3:AC:75:VAL:CB     | 2.29                     | 0.62              |
| 7:AG:92:SER:O      | 7:AG:96:GLN:HG3    | 2.00                     | 0.62              |
| 12:AL:47:LYS:HB3   | 12:AL:48:PRO:CD    | 2.29                     | 0.62              |
| 12:AL:6:THR:H      | 12:AL:9:GLN:NE2    | 1.89                     | 0.62              |
| 33:B8:51:ALA:N     | 33:B8:53:PRO:HD2   | 2.15                     | 0.62              |
| 35:BA:1216:G:HO2'  | 35:BA:1217:C:H5'   | 1.65                     | 0.62              |
| 35:BA:1227:G:N3    | 35:BA:1228:G:C8    | 2.68                     | 0.62              |
| 35:BA:2207:G:C2'   | 35:BA:2208:A:H5''  | 2.29                     | 0.62              |
| 35:BA:833:U:H4'    | 48:BP:52:GLU:N     | 2.15                     | 0.62              |
| 37:BC:125:GLY:O    | 37:BC:127:LYS:N    | 2.31                     | 0.62              |
| 35:BA:1803:A:H4'   | 38:BD:259:THR:HG23 | 1.82                     | 0.62              |
| 41:BG:164:GLU:HG3  | 41:BG:165:THR:H    | 1.65                     | 0.62              |
| 56:BX:40:LYS:HG2   | 56:BX:51:VAL:HB    | 1.82                     | 0.62              |
| 1:AA:1390:U:O2'    | 1:AA:1391:U:H5'    | 1.99                     | 0.62              |
| 1:AA:1492:A:C1'    | 1:AA:1493:A:OP1    | 2.45                     | 0.62              |
| 1:AA:775:G:C2'     | 1:AA:776:G:C5'     | 2.76                     | 0.62              |
| 10:AJ:4:ILE:CD1    | 10:AJ:77:PRO:HG3   | 2.28                     | 0.62              |
| 24:AY:539:ILE:O    | 24:AY:542:VAL:HG12 | 2.00                     | 0.62              |
| 27:B2:10:LEU:CD1   | 35:BA:78:A:OP1     | 2.48                     | 0.62              |
| 29:B4:12:ALA:O     | 29:B4:24:THR:CG2   | 2.43                     | 0.62              |
| 31:B6:15:GLU:HG2   | 31:B6:18:ARG:HH11  | 1.65                     | 0.62              |
| 35:BA:105:C:H2'    | 35:BA:106:C:C6     | 2.34                     | 0.62              |
| 35:BA:1428:C:N4    | 35:BA:1570:A:OP2   | 2.29                     | 0.62              |
| 35:BA:1999:C:C2'   | 35:BA:2000:G:C5'   | 2.71                     | 0.62              |
| 35:BA:221:A:C8     | 35:BA:266:G:O6     | 2.52                     | 0.62              |
| 38:BD:174:ILE:HG12 | 38:BD:184:LYS:HG2  | 1.82                     | 0.62              |
| 35:BA:2773:C:H5''  | 39:BE:164:ARG:HG2  | 1.82                     | 0.62              |
| 48:BP:24:GLY:N     | 48:BP:33:ARG:NE    | 2.47                     | 0.62              |
| 39:BE:52:LEU:HD11  | 52:BT:1:MET:CE     | 2.29                     | 0.62              |
| 52:BT:28:VAL:HG13  | 52:BT:29:ARG:H     | 1.60                     | 0.62              |
| 52:BT:58:ASN:H     | 52:BT:58:ASN:ND2   | 1.97                     | 0.62              |
| 57:BY:28:LYS:HA    | 57:BY:39:VAL:H     | 1.64                     | 0.62              |
| 1:AA:1047:G:C2'    | 1:AA:1048:G:C5'    | 2.72                     | 0.61              |
| 1:AA:1270:C:O2'    | 1:AA:1314:C:H5'    | 2.00                     | 0.61              |
| 1:AA:861:G:O2'     | 1:AA:862:C:H5'     | 2.00                     | 0.61              |
| 3:AC:64:VAL:HB     | 3:AC:99:VAL:HG12   | 1.82                     | 0.61              |
| 13:AM:40:ASN:HD22  | 13:AM:43:THR:HG23  | 1.64                     | 0.61              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 26:B1:40:ARG:NH2   | 26:B1:42:GLN:HG2    | 2.15                     | 0.61              |
| 32:B7:8:ASN:HD22   | 32:B7:9:ARG:N       | 1.98                     | 0.61              |
| 35:BA:1141:U:H4'   | 35:BA:1142(A):A:O4' | 2.00                     | 0.61              |
| 35:BA:1300:U:H5''  | 35:BA:1301:A:C2     | 2.35                     | 0.61              |
| 35:BA:262:A:H2'    | 35:BA:263:C:C5'     | 2.29                     | 0.61              |
| 35:BA:328:U:H6     | 35:BA:328:U:O5'     | 1.82                     | 0.61              |
| 35:BA:331:A:O2'    | 35:BA:332:A:P       | 2.58                     | 0.61              |
| 41:BG:101:ILE:HA   | 41:BG:105:LYS:HG2   | 1.82                     | 0.61              |
| 51:BS:89:ARG:HG2   | 51:BS:92:TYR:HA     | 1.83                     | 0.61              |
| 52:BT:58:ASN:H     | 52:BT:58:ASN:HD22   | 1.48                     | 0.61              |
| 54:BV:19:LYS:HB3   | 54:BV:94:LEU:O      | 2.00                     | 0.61              |
| 49:BQ:137:TYR:HE1  | 58:BZ:81:ARG:NH2    | 1.97                     | 0.61              |
| 1:AA:1015:A:H2'    | 1:AA:1016:A:C8      | 2.35                     | 0.61              |
| 3:AC:168:ALA:O     | 3:AC:169:ALA:CB     | 2.46                     | 0.61              |
| 5:AE:148:VAL:HG21  | 8:AH:107:LEU:HD13   | 1.82                     | 0.61              |
| 6:AF:4:TYR:CD1     | 6:AF:92:LYS:HA      | 2.35                     | 0.61              |
| 7:AG:47:CYS:SG     | 7:AG:48:LYS:N       | 2.73                     | 0.61              |
| 15:AO:82:ILE:HD13  | 15:AO:82:ILE:O      | 2.01                     | 0.61              |
| 25:B0:43:THR:HG22  | 35:BA:2331:G:O3'    | 1.99                     | 0.61              |
| 28:B3:22:ALA:HB3   | 28:B3:50:VAL:CG1    | 2.29                     | 0.61              |
| 35:BA:1065:U:H2'   | 35:BA:1067:A:OP1    | 1.99                     | 0.61              |
| 35:BA:12:U:O2      | 35:BA:2626:C:H4'    | 2.00                     | 0.61              |
| 35:BA:1798:U:C5'   | 38:BD:259:THR:HG22  | 2.29                     | 0.61              |
| 35:BA:2408:U:H2'   | 35:BA:2409:G:H8     | 1.65                     | 0.61              |
| 35:BA:271(A):A:H5' | 35:BA:271(B):C:OP2  | 2.00                     | 0.61              |
| 35:BA:548:A:H2'    | 35:BA:549:G:O4'     | 2.00                     | 0.61              |
| 35:BA:1820:U:C1'   | 38:BD:202:LYS:HB3   | 2.29                     | 0.61              |
| 39:BE:134:ILE:C    | 39:BE:134:ILE:CD1   | 2.68                     | 0.61              |
| 35:BA:674:G:O2'    | 40:BF:74:ARG:HD3    | 2.00                     | 0.61              |
| 41:BG:137:GLU:C    | 41:BG:138:GLN:HG2   | 2.20                     | 0.61              |
| 41:BG:11:TYR:O     | 41:BG:16:ARG:HB2    | 2.00                     | 0.61              |
| 41:BG:66:GLN:HE22  | 41:BG:94:LEU:CD2    | 2.13                     | 0.61              |
| 46:BN:3:THR:HG22   | 46:BN:4:TYR:N       | 2.14                     | 0.61              |
| 48:BP:6:LEU:N      | 48:BP:6:LEU:HD23    | 2.14                     | 0.61              |
| 57:BY:81:LYS:CB    | 57:BY:96:ILE:HD11   | 2.30                     | 0.61              |
| 1:AA:110:C:O2'     | 1:AA:111:G:H5'      | 2.00                     | 0.61              |
| 1:AA:1151:A:C2     | 1:AA:1152:A:C6      | 2.89                     | 0.61              |
| 1:AA:1286:A:O2'    | 1:AA:1287:A:H5''    | 1.98                     | 0.61              |
| 1:AA:1492:A:C1'    | 1:AA:1493:A:P       | 2.88                     | 0.61              |
| 1:AA:77:G:H1       | 1:AA:92:C:N4        | 1.99                     | 0.61              |
| 1:AA:975:A:H4'     | 1:AA:976:G:C5'      | 2.21                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:828:A:N3     | 2:AB:26:PRO:HG2    | 2.15                     | 0.61              |
| 9:AI:18:PHE:O     | 9:AI:61:ALA:C      | 2.39                     | 0.61              |
| 10:AJ:24:VAL:HG21 | 10:AJ:37:PRO:HG3   | 1.81                     | 0.61              |
| 15:AO:47:LYS:HD2  | 15:AO:47:LYS:H     | 1.64                     | 0.61              |
| 15:AO:54:ARG:HG2  | 15:AO:58:MET:HE2   | 1.82                     | 0.61              |
| 24:AY:127:LYS:HE3 | 24:AY:128:TYR:CE1  | 2.34                     | 0.61              |
| 24:AY:210:ARG:HG2 | 24:AY:210:ARG:HH11 | 1.65                     | 0.61              |
| 24:AY:100:VAL:CG2 | 24:AY:329:ARG:HB2  | 2.29                     | 0.61              |
| 24:AY:535:PRO:C   | 24:AY:537:GLU:H    | 2.03                     | 0.61              |
| 27:B2:33:MET:O    | 27:B2:37:PHE:HB2   | 1.99                     | 0.61              |
| 28:B3:1:MET:CB    | 28:B3:2:PRO:CD     | 2.77                     | 0.61              |
| 29:B4:42:PHE:CE1  | 41:BG:180:PHE:HE1  | 2.18                     | 0.61              |
| 33:B8:50:LEU:C    | 33:B8:53:PRO:HD2   | 2.20                     | 0.61              |
| 35:BA:1460:A:O2'  | 35:BA:1461:G:C5'   | 2.48                     | 0.61              |
| 35:BA:1599:C:O2'  | 35:BA:1600:C:H5'   | 2.01                     | 0.61              |
| 35:BA:2712:U:O2'  | 35:BA:2712(A):A:P  | 2.58                     | 0.61              |
| 35:BA:696:G:H2'   | 35:BA:697:C:H5'    | 1.81                     | 0.61              |
| 37:BC:103:LYS:NZ  | 37:BC:103:LYS:HA   | 2.15                     | 0.61              |
| 37:BC:127:LYS:N   | 37:BC:127:LYS:HD3  | 2.15                     | 0.61              |
| 46:BN:6:PRO:O     | 46:BN:7:LYS:HB3    | 2.00                     | 0.61              |
| 52:BT:11:GLU:CD   | 52:BT:11:GLU:N     | 2.53                     | 0.61              |
| 1:AA:1399:C:C5'   | 1:AA:1400:C:H3'    | 2.29                     | 0.61              |
| 1:AA:384:G:H2'    | 1:AA:385:C:C6      | 2.35                     | 0.61              |
| 1:AA:961:U:H3'    | 1:AA:961:U:OP1     | 2.01                     | 0.61              |
| 2:AB:15:VAL:O     | 2:AB:16:HIS:ND1    | 2.31                     | 0.61              |
| 2:AB:228:GLY:C    | 2:AB:229:VAL:CG2   | 2.62                     | 0.61              |
| 2:AB:27:LYS:HD2   | 2:AB:193:ASP:OD1   | 2.00                     | 0.61              |
| 2:AB:80:ILE:H     | 2:AB:80:ILE:HD12   | 1.66                     | 0.61              |
| 3:AC:191:THR:HG21 | 3:AC:193:TYR:CZ    | 2.35                     | 0.61              |
| 4:AD:148:VAL:HG12 | 4:AD:149:ALA:N     | 2.14                     | 0.61              |
| 5:AE:100:VAL:HG23 | 5:AE:107:ARG:NH2   | 2.15                     | 0.61              |
| 30:B5:55:ARG:HA   | 30:B5:55:ARG:NE    | 2.15                     | 0.61              |
| 34:B9:10:ILE:HD13 | 34:B9:34:GLN:NE2   | 2.15                     | 0.61              |
| 35:BA:1153:C:H2'  | 35:BA:1154:G:O4'   | 2.00                     | 0.61              |
| 35:BA:1474:C:H2'  | 35:BA:1475:G:H5''  | 1.81                     | 0.61              |
| 35:BA:1964:G:H4'  | 35:BA:1965:C:OP2   | 2.00                     | 0.61              |
| 35:BA:2062:A:H8   | 35:BA:2062:A:H5'   | 1.65                     | 0.61              |
| 35:BA:2185:C:O2'  | 35:BA:2186:G:H8    | 1.83                     | 0.61              |
| 35:BA:2359:C:N4   | 35:BA:2360:A:N6    | 2.49                     | 0.61              |
| 42:BH:89:ILE:HB   | 42:BH:162:ILE:HG22 | 1.83                     | 0.61              |
| 45:BL:113:UNK:C   | 45:BL:115:UNK:N    | 2.62                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:BP:51:PHE:CA    | 48:BP:52:GLU:HB2   | 2.30                     | 0.61              |
| 51:BS:42:ASP:O     | 51:BS:43:GLU:HB3   | 1.99                     | 0.61              |
| 1:AA:1048:G:N3     | 1:AA:1050:G:N7     | 2.49                     | 0.61              |
| 1:AA:1124:G:O2'    | 1:AA:1145:C:N4     | 2.33                     | 0.61              |
| 10:AJ:75:ILE:HG13  | 10:AJ:76:ASN:N     | 2.14                     | 0.61              |
| 33:B8:30:ARG:NH2   | 35:BA:2419:U:O4    | 2.34                     | 0.61              |
| 35:BA:118:A:H5'    | 35:BA:119:A:H8     | 1.65                     | 0.61              |
| 35:BA:1227:G:C2'   | 35:BA:1228:G:H5'   | 2.29                     | 0.61              |
| 35:BA:1600:C:C2'   | 35:BA:1601:G:H5'   | 2.30                     | 0.61              |
| 35:BA:2620:C:OP1   | 39:BE:153:GLY:N    | 2.34                     | 0.61              |
| 38:BD:248:SER:HB2  | 38:BD:249:PRO:CD   | 2.22                     | 0.61              |
| 40:BF:136:THR:HG23 | 40:BF:170:LEU:HD21 | 1.82                     | 0.61              |
| 41:BG:7:LEU:HD12   | 41:BG:104:GLU:CD   | 2.20                     | 0.61              |
| 41:BG:129:GLY:HA3  | 41:BG:169:ALA:CB   | 2.31                     | 0.61              |
| 46:BN:90:MET:O     | 46:BN:93:THR:O     | 2.19                     | 0.61              |
| 48:BP:115:LEU:HD23 | 48:BP:115:LEU:C    | 2.21                     | 0.61              |
| 50:BR:3:HIS:C      | 50:BR:5:LYS:H      | 2.02                     | 0.61              |
| 51:BS:34:HIS:HB2   | 51:BS:36:TYR:HE1   | 1.65                     | 0.61              |
| 52:BT:34:VAL:HG22  | 52:BT:39:ARG:CB    | 2.31                     | 0.61              |
| 53:BU:88:ILE:O     | 53:BU:90:VAL:N     | 2.33                     | 0.61              |
| 53:BU:91:ASP:O     | 53:BU:92:ARG:HB3   | 1.99                     | 0.61              |
| 1:AA:936:C:O2'     | 1:AA:937:A:C5'     | 2.30                     | 0.61              |
| 12:AL:45:PRO:HG2   | 12:AL:51:ALA:H     | 1.63                     | 0.61              |
| 13:AM:49:THR:O     | 13:AM:53:VAL:HG23  | 2.01                     | 0.61              |
| 19:AS:22:LEU:HD13  | 19:AS:26:GLY:HA2   | 1.82                     | 0.61              |
| 24:AY:276:VAL:HA   | 24:AY:280:LEU:HD23 | 1.81                     | 0.61              |
| 27:B2:35:LEU:O     | 27:B2:37:PHE:N     | 2.33                     | 0.61              |
| 27:B2:2:LYS:O      | 27:B2:6:VAL:HG23   | 1.99                     | 0.61              |
| 29:B4:31:ILE:HG12  | 29:B4:33:VAL:H     | 1.65                     | 0.61              |
| 30:B5:3:LYS:HD2    | 35:BA:747:U:OP2    | 2.00                     | 0.61              |
| 35:BA:1019:U:O2'   | 35:BA:1021:A:C2    | 2.52                     | 0.61              |
| 35:BA:1113:U:OP1   | 42:BH:1:MET:N      | 2.34                     | 0.61              |
| 35:BA:2126:A:O2'   | 35:BA:2127:G:P     | 2.59                     | 0.61              |
| 35:BA:2130:U:H6    | 35:BA:2130:U:O5'   | 1.83                     | 0.61              |
| 35:BA:2492:U:H2'   | 35:BA:2493:U:H6    | 1.65                     | 0.61              |
| 35:BA:654(C):G:H2' | 35:BA:654(D):G:H5' | 1.82                     | 0.61              |
| 38:BD:134:ARG:NH1  | 38:BD:135:PHE:HE1  | 1.98                     | 0.61              |
| 38:BD:8:PRO:HB3    | 38:BD:14:ARG:HB3   | 1.81                     | 0.61              |
| 42:BH:118:PRO:HG2  | 42:BH:121:ILE:HD12 | 1.81                     | 0.61              |
| 42:BH:144:VAL:O    | 42:BH:148:ILE:HG12 | 2.00                     | 0.61              |
| 1:AA:1285:A:O2'    | 1:AA:1286:A:P      | 2.57                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1286:A:O2'    | 1:AA:1287:A:C4'    | 2.48                     | 0.61              |
| 1:AA:1494:G:O2'    | 1:AA:1495:U:H5'    | 2.01                     | 0.61              |
| 1:AA:267:C:OP2     | 17:AQ:67:LYS:HD2   | 2.00                     | 0.61              |
| 1:AA:925:G:H1'     | 1:AA:1502:A:C4     | 2.35                     | 0.61              |
| 2:AB:54:THR:HG21   | 2:AB:201:ILE:HD11  | 1.81                     | 0.61              |
| 5:AE:147:ASP:HB3   | 5:AE:150:ARG:HH12  | 1.65                     | 0.61              |
| 10:AJ:50:ILE:HD11  | 10:AJ:57:LYS:HD3   | 1.82                     | 0.61              |
| 24:AY:252:ASP:O    | 24:AY:253:LEU:HB2  | 1.99                     | 0.61              |
| 24:AY:5:VAL:C      | 24:AY:7:TYR:H      | 2.04                     | 0.61              |
| 24:AY:681:LYS:O    | 24:AY:681:LYS:HD2  | 1.99                     | 0.61              |
| 32:B7:12:ARG:HD3   | 32:B7:46:VAL:HG21  | 1.82                     | 0.61              |
| 35:BA:1475:G:O2'   | 35:BA:1476:C:H5'   | 2.01                     | 0.61              |
| 35:BA:1810:A:O5'   | 35:BA:1810:A:H8    | 1.82                     | 0.61              |
| 35:BA:2031:A:O2'   | 35:BA:2454:G:N2    | 2.33                     | 0.61              |
| 35:BA:2317:C:C2'   | 35:BA:2318:G:H5'   | 2.31                     | 0.61              |
| 35:BA:271(U):G:O2' | 35:BA:271(V):G:H5' | 2.01                     | 0.61              |
| 35:BA:45:C:C2      | 35:BA:47:C:C5      | 2.89                     | 0.61              |
| 35:BA:622:G:O2'    | 35:BA:623:G:H5'    | 2.00                     | 0.61              |
| 36:BB:25:A:N3      | 36:BB:25:A:H2'     | 2.15                     | 0.61              |
| 40:BF:108:LYS:O    | 40:BF:112:MET:HG3  | 2.01                     | 0.61              |
| 41:BG:7:LEU:O      | 41:BG:10:LYS:N     | 2.33                     | 0.61              |
| 48:BP:125:VAL:O    | 48:BP:145:PRO:HD2  | 2.00                     | 0.61              |
| 49:BQ:61:GLY:O     | 49:BQ:62:GLY:O     | 2.18                     | 0.61              |
| 51:BS:42:ASP:C     | 51:BS:44:LYS:H     | 2.03                     | 0.61              |
| 56:BX:24:GLY:O     | 56:BX:82:GLN:HA    | 2.00                     | 0.61              |
| 58:BZ:156:LYS:O    | 58:BZ:158:PRO:HD3  | 2.00                     | 0.61              |
| 58:BZ:79:ARG:O     | 58:BZ:81:ARG:N     | 2.34                     | 0.61              |
| 1:AA:1354:C:O2'    | 1:AA:1355:G:H5'    | 2.01                     | 0.61              |
| 1:AA:590:C:O2'     | 1:AA:591:U:C5'     | 2.30                     | 0.61              |
| 2:AB:187:LEU:O     | 2:AB:187:LEU:CD1   | 2.48                     | 0.61              |
| 1:AA:542:G:OP1     | 4:AD:10:ARG:NH2    | 2.34                     | 0.61              |
| 13:AM:15:VAL:HG22  | 13:AM:41:PRO:O     | 2.01                     | 0.61              |
| 24:AY:198:GLU:HG3  | 24:AY:198:GLU:O    | 2.00                     | 0.61              |
| 30:B5:57:VAL:HG12  | 30:B5:58:LEU:N     | 2.12                     | 0.61              |
| 34:B9:35:ARG:O     | 34:B9:36:GLN:HB2   | 1.99                     | 0.61              |
| 35:BA:1417:C:H2'   | 35:BA:1418:G:H5'   | 1.76                     | 0.61              |
| 35:BA:175:G:O2'    | 35:BA:176:G:H5'    | 1.99                     | 0.61              |
| 35:BA:1995:U:H3'   | 35:BA:1996:C:H2'   | 1.82                     | 0.61              |
| 35:BA:2753:A:O2'   | 35:BA:2754:U:C5'   | 2.30                     | 0.61              |
| 36:BB:87:G:H2'     | 36:BB:88:C:H5"     | 1.81                     | 0.61              |
| 37:BC:117:THR:O    | 37:BC:147:GLY:O    | 2.19                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:BV:47:VAL:HG12  | 54:BV:52:VAL:HB    | 1.82                     | 0.61              |
| 1:AA:1305:G:N2     | 1:AA:1332:A:OP2    | 2.34                     | 0.61              |
| 1:AA:1457:G:H8     | 1:AA:1457:G:OP2    | 1.84                     | 0.61              |
| 1:AA:787:A:H2'     | 1:AA:788:U:H5'     | 1.82                     | 0.61              |
| 2:AB:189:ASP:HB3   | 2:AB:203:GLY:O     | 2.01                     | 0.61              |
| 4:AD:33:MET:O      | 4:AD:37:PRO:HG3    | 2.00                     | 0.61              |
| 13:AM:5:ALA:HB2    | 13:AM:66:LEU:HD22  | 1.82                     | 0.61              |
| 33:B8:43:GLN:O     | 33:B8:44:LYS:HD2   | 2.00                     | 0.61              |
| 35:BA:1204:A:N1    | 35:BA:1241:A:H2    | 1.98                     | 0.61              |
| 35:BA:1925:C:C3'   | 35:BA:1926:U:H5''  | 2.30                     | 0.61              |
| 35:BA:2359:C:N4    | 35:BA:2360:A:C6    | 2.68                     | 0.61              |
| 35:BA:2492:U:H2'   | 35:BA:2493:U:C6    | 2.35                     | 0.61              |
| 38:BD:70:TRP:HZ3   | 38:BD:146:GLU:OE2  | 1.83                     | 0.61              |
| 39:BE:141:ILE:HA   | 39:BE:154:LYS:CE   | 2.30                     | 0.61              |
| 40:BF:10:PRO:HA    | 40:BF:127:GLU:CB   | 2.31                     | 0.61              |
| 41:BG:118:ARG:NH1  | 41:BG:182:LYS:HD3  | 2.15                     | 0.61              |
| 1:AA:1193:G:C2'    | 1:AA:1194:U:H5'    | 2.30                     | 0.61              |
| 1:AA:119:A:HO2'    | 1:AA:120:A:P       | 2.23                     | 0.61              |
| 1:AA:1386:G:C2'    | 1:AA:1387:G:H5'    | 2.30                     | 0.61              |
| 8:AH:116:LYS:HD3   | 8:AH:127:LEU:HD12  | 1.82                     | 0.61              |
| 12:AL:18:VAL:CG2   | 12:AL:19:ARG:H     | 2.13                     | 0.61              |
| 24:AY:21:ILE:CD1   | 24:AY:21:ILE:H     | 2.12                     | 0.61              |
| 24:AY:191:ASP:CB   | 24:AY:265:LYS:HG3  | 2.27                     | 0.61              |
| 26:B1:89:GLU:HA    | 26:B1:92:LYS:HG2   | 1.83                     | 0.61              |
| 35:BA:1181:C:O2'   | 35:BA:1182:A:H5'   | 2.00                     | 0.61              |
| 35:BA:1646:C:H5''  | 35:BA:1647:G:H5''  | 1.79                     | 0.61              |
| 35:BA:1945:G:C5    | 35:BA:1946:U:C4    | 2.88                     | 0.61              |
| 35:BA:2787:C:H1'   | 39:BE:61:ARG:NH1   | 2.14                     | 0.61              |
| 35:BA:582:G:H2'    | 35:BA:583:G:C8     | 2.35                     | 0.61              |
| 35:BA:7:G:H2'      | 35:BA:8:A:O4'      | 2.01                     | 0.61              |
| 38:BD:248:SER:CB   | 38:BD:249:PRO:HD2  | 2.23                     | 0.61              |
| 35:BA:2620:C:C5'   | 39:BE:153:GLY:HA2  | 2.27                     | 0.61              |
| 39:BE:76:ARG:O     | 39:BE:77:ILE:O     | 2.19                     | 0.61              |
| 40:BF:183:VAL:O    | 40:BF:187:VAL:HG23 | 1.99                     | 0.61              |
| 50:BR:99:LYS:N     | 50:BR:99:LYS:HD2   | 2.11                     | 0.61              |
| 57:BY:96:ILE:CG2   | 57:BY:99:CYS:SG    | 2.89                     | 0.61              |
| 58:BZ:183:LEU:HD13 | 58:BZ:184:ALA:N    | 2.15                     | 0.61              |
| 1:AA:877:C:O2'     | 1:AA:878:G:H5'     | 2.01                     | 0.60              |
| 1:AA:957:U:H2'     | 1:AA:959:A:OP2     | 2.01                     | 0.60              |
| 2:AB:127:ILE:O     | 2:AB:127:ILE:HD13  | 2.01                     | 0.60              |
| 2:AB:187:LEU:C     | 2:AB:187:LEU:CD2   | 2.61                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:AI:22:GLY:N      | 9:AI:58:HIS:O     | 2.33                     | 0.60              |
| 12:AL:20:LYS:N     | 12:AL:20:LYS:HD3  | 2.16                     | 0.60              |
| 13:AM:116:THR:O    | 13:AM:117:VAL:HB  | 2.01                     | 0.60              |
| 17:AQ:68:ARG:H     | 17:AQ:70:ARG:NH1  | 1.99                     | 0.60              |
| 22:AV:45:U:O2      | 22:AV:45:U:C5'    | 2.49                     | 0.60              |
| 33:B8:6:THR:HA     | 33:B8:61:LEU:HD11 | 1.82                     | 0.60              |
| 34:B9:9:ARG:O      | 34:B9:14:CYS:SG   | 2.59                     | 0.60              |
| 35:BA:1107:G:OP1   | 43:BJ:58:UNK:HA   | 2.00                     | 0.60              |
| 35:BA:1445:A:H5'   | 35:BA:1460:A:H1'  | 1.83                     | 0.60              |
| 35:BA:1709:U:H2'   | 35:BA:1710:C:C6   | 2.36                     | 0.60              |
| 35:BA:1820:U:C2    | 38:BD:159:ALA:O   | 2.54                     | 0.60              |
| 38:BD:35:LYS:NZ    | 38:BD:35:LYS:CB   | 2.64                     | 0.60              |
| 51:BS:34:HIS:HB3   | 51:BS:53:SER:CB   | 2.29                     | 0.60              |
| 53:BU:86:ALA:HB2   | 53:BU:116:ALA:HB2 | 1.83                     | 0.60              |
| 57:BY:44:ILE:HG22  | 57:BY:45:VAL:H    | 1.64                     | 0.60              |
| 58:BZ:122:ARG:HH11 | 58:BZ:122:ARG:HB3 | 1.66                     | 0.60              |
| 1:AA:358:U:H2'     | 1:AA:359:U:C6     | 2.36                     | 0.60              |
| 1:AA:688:G:N1      | 1:AA:700:G:C5     | 2.68                     | 0.60              |
| 1:AA:874:G:C6      | 1:AA:875:C:C4     | 2.89                     | 0.60              |
| 5:AE:100:VAL:HG23  | 5:AE:107:ARG:HH21 | 1.65                     | 0.60              |
| 7:AG:22:LEU:HD21   | 7:AG:101:LEU:HD11 | 1.82                     | 0.60              |
| 9:AI:27:THR:HA     | 9:AI:31:GLN:O     | 2.01                     | 0.60              |
| 24:AY:201:ILE:H    | 24:AY:201:ILE:CD1 | 2.08                     | 0.60              |
| 24:AY:31:ARG:HH12  | 24:AY:34:TYR:HB3  | 1.67                     | 0.60              |
| 33:B8:32:LEU:CB    | 33:B8:36:LYS:NZ   | 2.64                     | 0.60              |
| 35:BA:1048:A:N6    | 42:BH:1:MET:HE1   | 2.15                     | 0.60              |
| 35:BA:1403:C:H5''  | 35:BA:1471:A:C1'  | 2.31                     | 0.60              |
| 35:BA:261:G:C2'    | 35:BA:262:A:H5'   | 2.30                     | 0.60              |
| 35:BA:271(Q):G:O2' | 35:BA:271(R):G:H8 | 1.84                     | 0.60              |
| 35:BA:896:A:H1'    | 58:BZ:176:PRO:CB  | 2.30                     | 0.60              |
| 37:BC:53:ARG:H     | 37:BC:53:ARG:HD3  | 1.65                     | 0.60              |
| 40:BF:42:ALA:O     | 40:BF:45:ARG:HG3  | 2.01                     | 0.60              |
| 51:BS:63:THR:O     | 51:BS:67:ARG:HG3  | 2.01                     | 0.60              |
| 58:BZ:128:VAL:CG2  | 58:BZ:129:SER:H   | 2.08                     | 0.60              |
| 58:BZ:183:LEU:HD11 | 58:BZ:186:GLU:N   | 2.16                     | 0.60              |
| 1:AA:1281:U:OP2    | 1:AA:1282:C:N4    | 2.34                     | 0.60              |
| 1:AA:1305:G:H1'    | 1:AA:1332:A:N6    | 2.16                     | 0.60              |
| 1:AA:1385:G:H2'    | 1:AA:1386:G:C8    | 2.36                     | 0.60              |
| 1:AA:189(H):G:O2'  | 1:AA:189(I):G:H8  | 1.83                     | 0.60              |
| 1:AA:501:C:H2'     | 1:AA:502:G:H8     | 1.66                     | 0.60              |
| 2:AB:27:LYS:O      | 2:AB:29:ALA:N     | 2.32                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B0:21:LEU:CD1   | 25:B0:41:ARG:HG2   | 2.31                     | 0.60              |
| 33:B8:27:THR:HG22  | 48:BP:62:LEU:HD22  | 1.82                     | 0.60              |
| 35:BA:1348:G:H2'   | 35:BA:1349:A:H5''  | 1.83                     | 0.60              |
| 35:BA:2356:C:H2'   | 35:BA:2357:U:O5'   | 2.00                     | 0.60              |
| 26:B1:25:LYS:HD3   | 35:BA:2396:G:H5'   | 1.82                     | 0.60              |
| 35:BA:2405:G:H8    | 35:BA:2405:G:O5'   | 1.85                     | 0.60              |
| 33:B8:30:ARG:CZ    | 35:BA:2419:U:O4    | 2.49                     | 0.60              |
| 35:BA:31:C:O2'     | 35:BA:32:C:H5''    | 2.00                     | 0.60              |
| 32:B7:37:LYS:HE2   | 35:BA:469:G:O6     | 2.01                     | 0.60              |
| 38:BD:68:LYS:HG3   | 38:BD:68:LYS:O     | 2.01                     | 0.60              |
| 39:BE:69:LYS:N     | 39:BE:69:LYS:HE2   | 2.15                     | 0.60              |
| 41:BG:7:LEU:HD12   | 41:BG:104:GLU:CG   | 2.31                     | 0.60              |
| 40:BF:116:ASP:OD2  | 48:BP:5:ASP:N      | 2.34                     | 0.60              |
| 52:BT:35:LYS:HE2   | 52:BT:41:ARG:HD2   | 1.82                     | 0.60              |
| 1:AA:1488:G:H2'    | 1:AA:1489:G:H8     | 1.66                     | 0.60              |
| 1:AA:199:G:H2'     | 1:AA:200:G:H8      | 1.66                     | 0.60              |
| 1:AA:313:A:O2'     | 1:AA:314:C:H5'     | 2.01                     | 0.60              |
| 1:AA:937:A:O2'     | 1:AA:938:A:H5'     | 2.00                     | 0.60              |
| 3:AC:118:GLN:O     | 3:AC:120:VAL:N     | 2.34                     | 0.60              |
| 9:AI:95:LYS:O      | 9:AI:98:PRO:HD2    | 2.00                     | 0.60              |
| 10:AJ:89:ASP:HB3   | 10:AJ:91:PRO:CD    | 2.31                     | 0.60              |
| 31:B6:10:LEU:HD23  | 31:B6:10:LEU:N     | 2.06                     | 0.60              |
| 35:BA:141:A:C8     | 35:BA:1408:C:O2'   | 2.52                     | 0.60              |
| 35:BA:1446:C:H5    | 35:BA:1466:G:N3    | 1.99                     | 0.60              |
| 35:BA:1528(A):A:N6 | 35:BA:1541:G:N2    | 2.45                     | 0.60              |
| 35:BA:1820:U:C4'   | 35:BA:1821:A:OP2   | 2.40                     | 0.60              |
| 35:BA:1894:C:O5'   | 35:BA:1894:C:H6    | 1.85                     | 0.60              |
| 35:BA:2298:A:H62   | 35:BA:2318:G:H8    | 1.47                     | 0.60              |
| 37:BC:121:MET:SD   | 37:BC:124:VAL:HG11 | 2.41                     | 0.60              |
| 37:BC:214:TYR:CE2  | 37:BC:224:ARG:HG2  | 2.37                     | 0.60              |
| 38:BD:186:HIS:HD2  | 38:BD:188:GLU:H    | 1.50                     | 0.60              |
| 38:BD:30:GLU:CG    | 38:BD:63:ARG:NH2   | 2.64                     | 0.60              |
| 40:BF:3:GLU:HB2    | 40:BF:24:LEU:HG    | 1.84                     | 0.60              |
| 40:BF:84:VAL:HG23  | 40:BF:85:GLY:N     | 2.16                     | 0.60              |
| 48:BP:122:PRO:HA   | 48:BP:141:ALA:O    | 2.01                     | 0.60              |
| 50:BR:97:VAL:HA    | 50:BR:113:LEU:O    | 2.02                     | 0.60              |
| 51:BS:92:TYR:CG    | 51:BS:93:LYS:N     | 2.65                     | 0.60              |
| 58:BZ:130:PRO:O    | 58:BZ:133:ILE:HG12 | 2.01                     | 0.60              |
| 2:AB:17:PHE:O      | 2:AB:17:PHE:HD1    | 1.83                     | 0.60              |
| 1:AA:1108:G:H5'    | 3:AC:176:HIS:CD2   | 2.35                     | 0.60              |
| 10:AJ:4:ILE:N      | 10:AJ:4:ILE:HD12   | 2.16                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:89:ASP:HB3   | 10:AJ:91:PRO:HD2   | 1.84                     | 0.60              |
| 11:AK:82:VAL:CG1   | 11:AK:108:ILE:HG12 | 2.31                     | 0.60              |
| 15:AO:26:GLU:OE2   | 15:AO:77:ARG:HD2   | 2.01                     | 0.60              |
| 19:AS:64:GLU:HB2   | 29:B4:48:ARG:NH2   | 2.16                     | 0.60              |
| 20:AT:96:GLY:O     | 20:AT:97:ALA:HB3   | 2.00                     | 0.60              |
| 27:B2:40:SER:O     | 56:BX:13:LEU:HD11  | 2.02                     | 0.60              |
| 29:B4:14:ILE:O     | 29:B4:15:ILE:C     | 2.39                     | 0.60              |
| 35:BA:1225:G:O2'   | 35:BA:1226:A:H5'   | 2.02                     | 0.60              |
| 35:BA:1769:G:C2'   | 35:BA:1770:G:H5'   | 2.31                     | 0.60              |
| 35:BA:1821:A:C2'   | 35:BA:1822:G:C5'   | 2.68                     | 0.60              |
| 35:BA:37:C:HO2'    | 35:BA:38:A:H5'     | 1.65                     | 0.60              |
| 37:BC:80:LYS:HE2   | 37:BC:99:GLU:HG2   | 1.84                     | 0.60              |
| 38:BD:232:PRO:HD2  | 38:BD:249:PRO:HA   | 1.83                     | 0.60              |
| 39:BE:134:ILE:O    | 39:BE:134:ILE:CD1  | 2.48                     | 0.60              |
| 41:BG:182:LYS:OXT  | 41:BG:182:LYS:HD2  | 2.02                     | 0.60              |
| 1:AA:1158:C:O2     | 1:AA:1181:G:N2     | 2.34                     | 0.60              |
| 1:AA:1170:A:H2'    | 1:AA:1171:G:O4'    | 2.02                     | 0.60              |
| 1:AA:167:G:O2'     | 1:AA:168:G:H5'     | 2.02                     | 0.60              |
| 1:AA:265:G:H2'     | 1:AA:266:G:C5'     | 2.18                     | 0.60              |
| 1:AA:328:C:H4'     | 1:AA:329:A:H5'     | 1.82                     | 0.60              |
| 1:AA:563:A:O2'     | 1:AA:566:G:O3'     | 2.19                     | 0.60              |
| 2:AB:106:LYS:O     | 2:AB:110:GLN:HB3   | 2.02                     | 0.60              |
| 24:AY:8:ASP:O      | 24:AY:9:LEU:HB3    | 1.99                     | 0.60              |
| 29:B4:6:HIS:CE1    | 41:BG:66:GLN:HB2   | 2.37                     | 0.60              |
| 35:BA:1067:A:H5''  | 35:BA:1068:G:C5'   | 2.28                     | 0.60              |
| 35:BA:1422:G:C6    | 35:BA:1423:G:C6    | 2.90                     | 0.60              |
| 35:BA:1864:U:H2'   | 35:BA:1865:G:H5''  | 1.83                     | 0.60              |
| 35:BA:947:G:H2'    | 35:BA:948:G:C8     | 2.36                     | 0.60              |
| 39:BE:134:ILE:O    | 39:BE:134:ILE:HD13 | 2.02                     | 0.60              |
| 40:BF:132:VAL:HG13 | 40:BF:133:ASN:ND2  | 2.16                     | 0.60              |
| 46:BN:12:ARG:NH2   | 46:BN:135:PRO:HG2  | 2.13                     | 0.60              |
| 48:BP:85:LEU:HD23  | 48:BP:117:GLU:O    | 1.91                     | 0.60              |
| 51:BS:97:ARG:O     | 51:BS:99:LYS:HG3   | 2.01                     | 0.60              |
| 58:BZ:17:ALA:O     | 58:BZ:20:ARG:HG2   | 2.00                     | 0.60              |
| 1:AA:1279:A:O2'    | 1:AA:1282:C:N4     | 2.34                     | 0.60              |
| 1:AA:1321:C:H5''   | 1:AA:1322:C:C5'    | 2.32                     | 0.60              |
| 1:AA:328:C:O2      | 1:AA:328:C:H2'     | 2.01                     | 0.60              |
| 1:AA:490:G:C2'     | 1:AA:491:G:C5'     | 2.80                     | 0.60              |
| 1:AA:545:C:C3'     | 1:AA:546:G:H5'     | 2.32                     | 0.60              |
| 1:AA:755:G:OP2     | 15:AO:65:ARG:HD2   | 2.02                     | 0.60              |
| 1:AA:796:C:H2'     | 1:AA:797:C:H6      | 1.67                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:124:ILE:HD11  | 3:AC:196:LEU:HG    | 1.84                     | 0.60              |
| 10:AJ:78:ASN:HD22  | 10:AJ:80:LYS:N     | 1.95                     | 0.60              |
| 10:AJ:80:LYS:NZ    | 10:AJ:80:LYS:HB3   | 2.16                     | 0.60              |
| 10:AJ:96:ILE:HD13  | 10:AJ:96:ILE:H     | 1.66                     | 0.60              |
| 24:AY:227:ILE:HG23 | 24:AY:237:PRO:CG   | 2.30                     | 0.60              |
| 25:B0:4:LYS:HD3    | 35:BA:2252:G:O6    | 2.01                     | 0.60              |
| 29:B4:38:LYS:C     | 29:B4:38:LYS:HD2   | 2.22                     | 0.60              |
| 35:BA:15:G:C2'     | 35:BA:16:G:C5'     | 2.69                     | 0.60              |
| 35:BA:258:G:O2'    | 35:BA:259:G:H5'    | 2.01                     | 0.60              |
| 35:BA:2653:U:H5'   | 35:BA:2654:A:OP2   | 2.02                     | 0.60              |
| 35:BA:2808:U:O2'   | 35:BA:2809:A:H5'   | 2.01                     | 0.60              |
| 35:BA:652:C:C6     | 35:BA:653:A:N7     | 2.70                     | 0.60              |
| 35:BA:654(A):G:H2' | 35:BA:654(B):C:H5' | 1.83                     | 0.60              |
| 37:BC:121:MET:CE   | 37:BC:139:PRO:O    | 2.49                     | 0.60              |
| 37:BC:68:GLY:H     | 37:BC:189:ASN:HD21 | 1.47                     | 0.60              |
| 41:BG:103:LEU:HD11 | 41:BG:107:LEU:HG   | 1.84                     | 0.60              |
| 41:BG:88:ILE:O     | 41:BG:88:ILE:HG22  | 2.02                     | 0.60              |
| 50:BR:99:LYS:CD    | 50:BR:99:LYS:H     | 2.08                     | 0.60              |
| 56:BX:8:ILE:HD12   | 56:BX:8:ILE:H      | 1.66                     | 0.60              |
| 57:BY:101:LYS:CG   | 57:BY:102:CYS:N    | 2.56                     | 0.60              |
| 1:AA:1154:G:C2'    | 1:AA:1155:G:H5'    | 2.31                     | 0.60              |
| 1:AA:1179:A:C2'    | 1:AA:1180:A:C5'    | 2.79                     | 0.60              |
| 1:AA:1286:A:C2     | 21:AU:18:TYR:OH    | 2.54                     | 0.60              |
| 1:AA:1387:G:C6     | 1:AA:1388:C:N4     | 2.69                     | 0.60              |
| 1:AA:89:C:O2       | 1:AA:89:C:H2'      | 2.00                     | 0.60              |
| 1:AA:936:C:O5'     | 1:AA:936:C:H6      | 1.85                     | 0.60              |
| 1:AA:979:C:C3'     | 1:AA:980:C:H5''    | 2.32                     | 0.60              |
| 13:AM:23:TYR:HE2   | 13:AM:70:LEU:HD22  | 1.67                     | 0.60              |
| 15:AO:9:GLN:O      | 15:AO:13:GLN:HG3   | 2.01                     | 0.60              |
| 25:B0:27:GLU:OE1   | 25:B0:27:GLU:N     | 2.34                     | 0.60              |
| 26:B1:29:GLY:HA3   | 35:BA:2396:G:HO2'  | 1.63                     | 0.60              |
| 26:B1:90:ILE:O     | 26:B1:94:LEU:HD13  | 2.01                     | 0.60              |
| 27:B2:35:LEU:O     | 27:B2:38:GLN:N     | 2.32                     | 0.60              |
| 32:B7:10:ARG:O     | 32:B7:14:LYS:HG2   | 2.02                     | 0.60              |
| 35:BA:1865:G:C8    | 35:BA:1865:G:H5'   | 2.31                     | 0.60              |
| 35:BA:2633:G:H1'   | 39:BE:61:ARG:HD2   | 1.84                     | 0.60              |
| 35:BA:2682:U:H5'   | 35:BA:2682:U:H6    | 1.67                     | 0.60              |
| 35:BA:274:G:OP2    | 35:BA:274:G:H3'    | 2.00                     | 0.60              |
| 35:BA:676:A:H8     | 35:BA:2069:G:N2    | 1.86                     | 0.60              |
| 42:BH:83:TYR:HB3   | 42:BH:135:GLY:N    | 2.17                     | 0.60              |
| 42:BH:153:LYS:HG3  | 42:BH:154:PRO:HD2  | 1.83                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:BH:89:ILE:HD13  | 42:BH:94:TYR:HB3  | 1.83                     | 0.60              |
| 48:BP:146:VAL:HG13 | 48:BP:147:LEU:N   | 2.17                     | 0.60              |
| 49:BQ:56:ARG:HH11  | 49:BQ:56:ARG:CG   | 2.15                     | 0.60              |
| 56:BX:8:ILE:CD1    | 56:BX:42:ALA:HB1  | 2.30                     | 0.60              |
| 1:AA:1037:C:H2'    | 1:AA:1038:C:C2    | 2.36                     | 0.60              |
| 1:AA:109:A:N6      | 1:AA:326:G:C6     | 2.69                     | 0.60              |
| 1:AA:1285:A:O4'    | 1:AA:1286:A:C8    | 2.55                     | 0.60              |
| 3:AC:50:ALA:CB     | 3:AC:75:VAL:HB    | 2.31                     | 0.60              |
| 7:AG:49:ILE:HD12   | 7:AG:121:ALA:HB3  | 1.84                     | 0.60              |
| 8:AH:116:LYS:HD2   | 8:AH:129:VAL:HG11 | 1.84                     | 0.60              |
| 13:AM:97:PRO:HA    | 13:AM:110:ARG:HD3 | 1.83                     | 0.60              |
| 16:AP:58:TYR:O     | 16:AP:62:VAL:HG22 | 2.01                     | 0.60              |
| 24:AY:293:THR:HB   | 24:AY:294:PRO:HD2 | 1.82                     | 0.60              |
| 24:AY:99:ARG:NH1   | 24:AY:402:ILE:N   | 2.46                     | 0.60              |
| 24:AY:61:ARG:HB3   | 35:BA:2663:G:OP1  | 2.02                     | 0.60              |
| 29:B4:28:LYS:HE3   | 41:BG:145:THR:OG1 | 2.00                     | 0.60              |
| 31:B6:15:GLU:O     | 31:B6:17:LYS:N    | 2.31                     | 0.60              |
| 33:B8:25:MET:HG3   | 48:BP:64:LYS:HD3  | 1.84                     | 0.60              |
| 33:B8:50:LEU:O     | 33:B8:51:ALA:HB3  | 2.02                     | 0.60              |
| 35:BA:1119:C:H2'   | 35:BA:1120:G:H8   | 1.67                     | 0.60              |
| 26:B1:41:ARG:NH2   | 35:BA:1365:A:OP1  | 2.34                     | 0.60              |
| 35:BA:2409:G:C2'   | 35:BA:2410:G:H5'  | 2.31                     | 0.60              |
| 35:BA:221:A:C5     | 35:BA:266:G:N7    | 2.70                     | 0.60              |
| 35:BA:1819:A:OP1   | 38:BD:158:ALA:CB  | 2.49                     | 0.60              |
| 35:BA:1797:C:O2'   | 38:BD:259:THR:CG2 | 2.50                     | 0.60              |
| 38:BD:28:GLU:HB2   | 38:BD:29:PRO:CD   | 2.32                     | 0.60              |
| 40:BF:164:ARG:HH11 | 40:BF:164:ARG:HG2 | 1.67                     | 0.60              |
| 36:BB:56:G:C5'     | 41:BG:27:ASN:ND2  | 2.65                     | 0.60              |
| 53:BU:106:PHE:O    | 53:BU:109:LEU:HB2 | 2.01                     | 0.60              |
| 54:BV:15:GLU:O     | 54:BV:18:LEU:HD13 | 2.02                     | 0.60              |
| 1:AA:198:G:N1      | 1:AA:220:G:C4     | 2.69                     | 0.60              |
| 1:AA:197:A:C6      | 1:AA:221:C:C5'    | 2.85                     | 0.60              |
| 1:AA:438:G:O2'     | 1:AA:494:U:O4     | 2.19                     | 0.60              |
| 16:AP:66:PRO:HD2   | 16:AP:71:ARG:HH12 | 1.67                     | 0.60              |
| 26:B1:21:ARG:HG2   | 26:B1:22:GLY:N    | 2.16                     | 0.60              |
| 27:B2:16:LEU:HD22  | 27:B2:20:GLU:CB   | 2.29                     | 0.60              |
| 29:B4:2:LYS:CE     | 29:B4:5:ILE:HB    | 2.19                     | 0.60              |
| 34:B9:19:ARG:NH1   | 35:BA:2755:C:C4   | 2.70                     | 0.60              |
| 35:BA:1113:U:H2'   | 35:BA:1114:G:C8   | 2.37                     | 0.60              |
| 35:BA:1297:C:H2'   | 35:BA:1298:C:C6   | 2.37                     | 0.60              |
| 35:BA:1837:C:H2'   | 35:BA:1838:C:H5'' | 1.82                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1925:C:C4    | 35:BA:1926:U:C5    | 2.90                     | 0.60              |
| 35:BA:2127:G:C2'   | 35:BA:2128:C:C5'   | 2.79                     | 0.60              |
| 35:BA:2580:U:H4'   | 39:BE:130:GLY:CA   | 2.32                     | 0.60              |
| 35:BA:644:A:C2     | 35:BA:2369:A:H1'   | 2.36                     | 0.60              |
| 35:BA:654(V):A:OP2 | 35:BA:655:A:H3'    | 2.02                     | 0.60              |
| 35:BA:886:C:H3'    | 35:BA:887:A:H5''   | 1.83                     | 0.60              |
| 35:BA:995:C:C2     | 46:BN:1:MET:HG2    | 2.37                     | 0.60              |
| 36:BB:21:G:H2'     | 36:BB:22:U:O4'     | 2.01                     | 0.60              |
| 39:BE:167:VAL:HG22 | 39:BE:170:LEU:HD11 | 1.83                     | 0.60              |
| 49:BQ:70:PRO:HA    | 49:BQ:94:VAL:O     | 2.01                     | 0.60              |
| 50:BR:84:ALA:HB3   | 50:BR:85:PRO:HD3   | 1.82                     | 0.60              |
| 52:BT:39:ARG:HD2   | 52:BT:39:ARG:H     | 1.67                     | 0.60              |
| 57:BY:73:ARG:NH2   | 57:BY:82:PRO:HD3   | 2.16                     | 0.60              |
| 57:BY:88:LYS:HZ1   | 57:BY:93:GLY:HA3   | 1.66                     | 0.60              |
| 1:AA:1079:G:H2'    | 1:AA:1080:A:C8     | 2.37                     | 0.59              |
| 1:AA:1306:A:C2'    | 1:AA:1307:U:H5'    | 2.32                     | 0.59              |
| 1:AA:592:G:C2      | 1:AA:593:G:N7      | 2.70                     | 0.59              |
| 1:AA:639:G:O2'     | 1:AA:640:A:H5'     | 2.02                     | 0.59              |
| 2:AB:41:ILE:CG2    | 2:AB:41:ILE:O      | 2.50                     | 0.59              |
| 5:AE:144:THR:O     | 5:AE:148:VAL:HG23  | 2.01                     | 0.59              |
| 6:AF:19:LEU:HD23   | 6:AF:19:LEU:C      | 2.23                     | 0.59              |
| 7:AG:47:CYS:O      | 7:AG:51:GLN:N      | 2.35                     | 0.59              |
| 24:AY:554:PRO:HG2  | 24:AY:555:LEU:H    | 1.66                     | 0.59              |
| 24:AY:526:VAL:CG1  | 24:AY:566:THR:HG23 | 2.32                     | 0.59              |
| 25:B0:50:ASN:HB3   | 25:B0:63:VAL:HG22  | 1.83                     | 0.59              |
| 30:B5:7:PRO:HG2    | 35:BA:2016:U:O2    | 2.02                     | 0.59              |
| 35:BA:1106:G:C2'   | 35:BA:1107:G:C5'   | 2.78                     | 0.59              |
| 35:BA:1106:G:HO2'  | 35:BA:1107:G:H5'   | 1.66                     | 0.59              |
| 35:BA:1264:G:H2'   | 35:BA:2014:A:N6    | 2.16                     | 0.59              |
| 35:BA:2128:C:H1'   | 35:BA:2129:C:H5''  | 1.83                     | 0.59              |
| 33:B8:32:LEU:CD2   | 35:BA:2392:A:OP1   | 2.49                     | 0.59              |
| 35:BA:61:G:H1      | 35:BA:94:C:H42     | 1.49                     | 0.59              |
| 37:BC:121:MET:SD   | 37:BC:124:VAL:CG1  | 2.89                     | 0.59              |
| 35:BA:784:A:C5     | 38:BD:229:VAL:HG21 | 2.37                     | 0.59              |
| 39:BE:37:ARG:HA    | 39:BE:42:ASP:OD2   | 2.02                     | 0.59              |
| 39:BE:44:TYR:O     | 39:BE:45:THR:HB    | 2.02                     | 0.59              |
| 41:BG:159:VAL:HG13 | 41:BG:159:VAL:O    | 2.03                     | 0.59              |
| 41:BG:59:GLU:O     | 41:BG:63:ILE:HG23  | 2.02                     | 0.59              |
| 42:BH:143:GLN:HE22 | 42:BH:147:ASN:HD21 | 1.48                     | 0.59              |
| 42:BH:85:LYS:CE    | 42:BH:145:ALA:HB1  | 2.32                     | 0.59              |
| 1:AA:1049:U:HO2'   | 14:AN:2:ALA:N      | 2.00                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1308:U:OP1    | 13:AM:98:VAL:HG22  | 2.02                     | 0.59              |
| 1:AA:629:G:H2'     | 1:AA:630:G:O4'     | 2.02                     | 0.59              |
| 2:AB:88:ALA:HB2    | 2:AB:219:VAL:HG13  | 1.83                     | 0.59              |
| 3:AC:108:ASN:OD1   | 3:AC:110:ASN:ND2   | 2.35                     | 0.59              |
| 3:AC:130:VAL:O     | 3:AC:131:ARG:CB    | 2.50                     | 0.59              |
| 7:AG:49:ILE:CD1    | 7:AG:121:ALA:HB3   | 2.32                     | 0.59              |
| 13:AM:11:ARG:O     | 13:AM:13:LYS:N     | 2.35                     | 0.59              |
| 24:AY:637:ARG:HD2  | 24:AY:642:VAL:HG21 | 1.84                     | 0.59              |
| 27:B2:44:LEU:HD13  | 27:B2:45:SER:CA    | 2.32                     | 0.59              |
| 35:BA:1516:C:H2'   | 35:BA:1517:G:C5'   | 2.32                     | 0.59              |
| 35:BA:15:G:N3      | 35:BA:16:G:C8      | 2.70                     | 0.59              |
| 35:BA:176:G:H2'    | 35:BA:177:G:C5'    | 2.22                     | 0.59              |
| 35:BA:18:C:O2'     | 35:BA:19:C:H5'     | 2.02                     | 0.59              |
| 35:BA:2746:U:O2'   | 35:BA:2747:G:H5'   | 2.02                     | 0.59              |
| 35:BA:49:A:H5''    | 35:BA:51:G:C4'     | 2.32                     | 0.59              |
| 35:BA:676:A:H2     | 35:BA:802:A:H61    | 1.49                     | 0.59              |
| 35:BA:947:G:H2'    | 35:BA:948:G:H8     | 1.66                     | 0.59              |
| 37:BC:103:LYS:HZ1  | 37:BC:103:LYS:HA   | 1.67                     | 0.59              |
| 38:BD:71:ASP:HB2   | 38:BD:103:ARG:HH22 | 1.67                     | 0.59              |
| 40:BF:185:ASP:OD1  | 40:BF:188:ARG:NH1  | 2.34                     | 0.59              |
| 53:BU:92:ARG:NH2   | 54:BV:11:GLN:H     | 2.00                     | 0.59              |
| 1:AA:1288:A:O5'    | 1:AA:1288:A:H8     | 1.85                     | 0.59              |
| 1:AA:788:U:H2'     | 1:AA:789:U:C5'     | 2.31                     | 0.59              |
| 12:AL:113:ARG:O    | 12:AL:114:LYS:HD2  | 2.01                     | 0.59              |
| 19:AS:44:MET:HA    | 19:AS:44:MET:HE2   | 1.83                     | 0.59              |
| 22:AV:43:C:O2      | 22:AV:43:C:O4'     | 2.20                     | 0.59              |
| 29:B4:4:GLY:O      | 29:B4:5:ILE:HB     | 2.02                     | 0.59              |
| 31:B6:15:GLU:OE1   | 31:B6:18:ARG:CD    | 2.51                     | 0.59              |
| 35:BA:1087:G:H21   | 35:BA:1103:A:N6    | 1.99                     | 0.59              |
| 35:BA:1106:G:H2'   | 35:BA:1107:G:C5'   | 2.32                     | 0.59              |
| 35:BA:1301:A:C2'   | 35:BA:1302:A:H2'   | 2.31                     | 0.59              |
| 35:BA:1503:U:H2'   | 35:BA:1504:C:H6    | 1.64                     | 0.59              |
| 35:BA:1529:G:C2    | 35:BA:1541:G:N2    | 2.71                     | 0.59              |
| 35:BA:1571:A:H2'   | 35:BA:1572:A:C8    | 2.37                     | 0.59              |
| 35:BA:1805:U:H2'   | 35:BA:1806:C:H5'   | 1.83                     | 0.59              |
| 35:BA:1663:C:N4    | 35:BA:1998:G:O6    | 2.35                     | 0.59              |
| 35:BA:2312:U:OP1   | 41:BG:74:LYS:HG2   | 2.02                     | 0.59              |
| 25:B0:55:ARG:HD3   | 35:BA:2384:G:OP2   | 2.03                     | 0.59              |
| 35:BA:483:A:H5''   | 57:BY:49:VAL:HG22  | 1.83                     | 0.59              |
| 35:BA:654(E):G:H2' | 35:BA:654(F):C:O4' | 2.02                     | 0.59              |
| 35:BA:755:C:H2'    | 35:BA:756:C:C6     | 2.37                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:BC:122:GLY:O    | 37:BC:127:LYS:HE2 | 2.02                     | 0.59              |
| 41:BG:113:ARG:HA   | 41:BG:113:ARG:NE  | 2.17                     | 0.59              |
| 44:BK:41:UNK:C     | 44:BK:43:UNK:H    | 2.14                     | 0.59              |
| 48:BP:107:LYS:O    | 48:BP:109:GLY:N   | 2.36                     | 0.59              |
| 53:BU:59:ARG:HH11  | 53:BU:59:ARG:HG2  | 1.67                     | 0.59              |
| 57:BY:17:SER:CB    | 57:BY:71:LYS:HE2  | 2.32                     | 0.59              |
| 57:BY:26:LYS:O     | 57:BY:28:LYS:HE2  | 2.03                     | 0.59              |
| 1:AA:1049:U:H4'    | 1:AA:1050:G:H5'   | 1.82                     | 0.59              |
| 1:AA:326:G:O5'     | 1:AA:326:G:H8     | 1.85                     | 0.59              |
| 1:AA:397:A:N7      | 1:AA:548:G:OP2    | 2.35                     | 0.59              |
| 1:AA:522:C:H41     | 12:AL:53:ARG:HH21 | 1.46                     | 0.59              |
| 1:AA:865:A:O5'     | 1:AA:865:A:H8     | 1.83                     | 0.59              |
| 1:AA:946:A:C6      | 1:AA:947:G:C6     | 2.91                     | 0.59              |
| 2:AB:97:TRP:CZ3    | 2:AB:176:GLU:OE2  | 2.55                     | 0.59              |
| 5:AE:69:VAL:O      | 5:AE:71:LEU:N     | 2.35                     | 0.59              |
| 19:AS:40:ILE:HG22  | 19:AS:69:HIS:O    | 2.01                     | 0.59              |
| 24:AY:688:ILE:HG22 | 24:AY:688:ILE:O   | 2.02                     | 0.59              |
| 26:B1:82:LEU:O     | 26:B1:83:GLU:HB3  | 2.03                     | 0.59              |
| 27:B2:46:GLN:O     | 27:B2:47:ASN:C    | 2.41                     | 0.59              |
| 35:BA:1578:U:O2'   | 35:BA:1579:A:H5'' | 2.02                     | 0.59              |
| 35:BA:1652:A:N6    | 35:BA:1653:G:N1   | 2.51                     | 0.59              |
| 35:BA:178:G:O2'    | 35:BA:179:G:H5'   | 2.02                     | 0.59              |
| 35:BA:1822:G:C2'   | 35:BA:1823:G:H5'  | 2.30                     | 0.59              |
| 35:BA:1887:C:C2'   | 35:BA:1888:G:H5'' | 2.32                     | 0.59              |
| 35:BA:2469:A:H2'   | 35:BA:2470:G:C5'  | 2.29                     | 0.59              |
| 35:BA:28:A:H61     | 35:BA:512:G:H1'   | 1.65                     | 0.59              |
| 35:BA:476:G:H4'    | 35:BA:502:A:N1    | 2.18                     | 0.59              |
| 37:BC:89:GLU:C     | 37:BC:91:GLY:H    | 2.06                     | 0.59              |
| 41:BG:132:ASN:OD1  | 41:BG:158:ALA:HA  | 2.02                     | 0.59              |
| 41:BG:133:LEU:HD13 | 41:BG:134:GLY:H   | 1.66                     | 0.59              |
| 42:BH:169:VAL:HG13 | 42:BH:170:ARG:N   | 2.18                     | 0.59              |
| 43:BJ:27:UNK:CB    | 43:BJ:113:UNK:HA  | 2.32                     | 0.59              |
| 47:BO:9:GLU:HG3    | 47:BO:18:LYS:HZ2  | 1.67                     | 0.59              |
| 48:BP:23:PRO:HB2   | 48:BP:33:ARG:HG2  | 1.82                     | 0.59              |
| 51:BS:83:LYS:O     | 51:BS:105:ALA:HB3 | 2.02                     | 0.59              |
| 1:AA:359:U:H2'     | 1:AA:360:A:H8     | 1.66                     | 0.59              |
| 1:AA:512:U:H2'     | 1:AA:513:C:C6     | 2.38                     | 0.59              |
| 1:AA:563:A:O4'     | 1:AA:566:G:N3     | 2.36                     | 0.59              |
| 2:AB:24:TRP:CE3    | 2:AB:32:ILE:CD1   | 2.84                     | 0.59              |
| 4:AD:205:GLU:OE2   | 5:AE:100:VAL:HG22 | 2.02                     | 0.59              |
| 7:AG:15:ASP:OD1    | 7:AG:44:TYR:OH    | 2.20                     | 0.59              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:AY:5:VAL:O      | 24:AY:7:TYR:N       | 2.34                     | 0.59              |
| 24:AY:616:TYR:HE2  | 24:AY:664:GLN:HG3   | 1.66                     | 0.59              |
| 24:AY:81:ILE:O     | 24:AY:82:ILE:HG13   | 2.02                     | 0.59              |
| 29:B4:43:TYR:C     | 29:B4:45:GLY:N      | 2.56                     | 0.59              |
| 35:BA:1445:A:O4'   | 35:BA:1460:A:N3     | 2.36                     | 0.59              |
| 35:BA:1999:C:O5'   | 35:BA:1999:C:H6     | 1.85                     | 0.59              |
| 37:BC:194:ILE:HD11 | 37:BC:227:PRO:CB    | 2.32                     | 0.59              |
| 37:BC:41:THR:HG22  | 37:BC:42:VAL:N      | 2.17                     | 0.59              |
| 40:BF:20:LEU:H     | 40:BF:24:LEU:HD21   | 1.67                     | 0.59              |
| 41:BG:107:LEU:HD23 | 41:BG:111:LEU:HD11  | 1.84                     | 0.59              |
| 41:BG:146:TYR:O    | 41:BG:147:ASP:HB2   | 2.02                     | 0.59              |
| 46:BN:56:ASN:H     | 46:BN:125:GLY:HA3   | 1.68                     | 0.59              |
| 47:BO:18:LYS:HD2   | 47:BO:45:GLU:OE1    | 2.02                     | 0.59              |
| 33:B8:13:ARG:CD    | 48:BP:61:ARG:HD2    | 2.24                     | 0.59              |
| 51:BS:78:LEU:HD11  | 51:BS:103:GLU:HB2   | 1.83                     | 0.59              |
| 54:BV:39:LEU:HA    | 54:BV:47:VAL:HG13   | 1.84                     | 0.59              |
| 58:BZ:5:LEU:O      | 58:BZ:59:LEU:HA     | 2.01                     | 0.59              |
| 1:AA:1005:A:C2'    | 1:AA:1006:C:H5'     | 2.33                     | 0.59              |
| 1:AA:1281:U:H4'    | 1:AA:1282:C:OP2     | 2.02                     | 0.59              |
| 1:AA:1286:A:O2'    | 1:AA:1287:A:P       | 2.60                     | 0.59              |
| 1:AA:519:C:N4      | 1:AA:520:A:C6       | 2.71                     | 0.59              |
| 1:AA:530:G:H3'     | 1:AA:531:U:C5'      | 2.33                     | 0.59              |
| 1:AA:941:G:C2'     | 1:AA:942:G:O5'      | 2.51                     | 0.59              |
| 1:AA:961:U:C2'     | 1:AA:962:C:H5'      | 2.33                     | 0.59              |
| 2:AB:204:ASN:HD21  | 2:AB:206:ASP:H      | 1.47                     | 0.59              |
| 4:AD:120:LEU:HB3   | 4:AD:126:ILE:CD1    | 2.32                     | 0.59              |
| 7:AG:16:LEU:HD12   | 9:AI:42:ARG:HA      | 1.83                     | 0.59              |
| 12:AL:27:LEU:CD1   | 12:AL:28:LYS:HE2    | 2.25                     | 0.59              |
| 12:AL:47:LYS:HB3   | 12:AL:48:PRO:HD3    | 1.82                     | 0.59              |
| 16:AP:18:ARG:HD3   | 16:AP:35:LYS:HD2    | 1.84                     | 0.59              |
| 24:AY:25:LYS:HZ2   | 24:AY:86:GLY:N      | 1.98                     | 0.59              |
| 33:B8:50:LEU:HD12  | 33:B8:51:ALA:N      | 2.17                     | 0.59              |
| 35:BA:1027:A:N6    | 35:BA:1126:A:C4     | 2.70                     | 0.59              |
| 35:BA:1445:A:O2'   | 35:BA:1445(A):C:H5' | 2.02                     | 0.59              |
| 35:BA:1504:C:O2'   | 35:BA:1505:C:H5'    | 2.02                     | 0.59              |
| 35:BA:1517:G:H5'   | 35:BA:1517:G:C8     | 2.34                     | 0.59              |
| 35:BA:1639:U:H2'   | 35:BA:1640:C:H5''   | 1.83                     | 0.59              |
| 35:BA:1267:U:C5    | 35:BA:2012:G:N2     | 2.70                     | 0.59              |
| 35:BA:2201:C:HO2'  | 35:BA:2202:C:H5'    | 1.61                     | 0.59              |
| 35:BA:651:G:C6     | 35:BA:652:C:N4      | 2.71                     | 0.59              |
| 37:BC:214:TYR:CZ   | 37:BC:224:ARG:HG2   | 2.37                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:BP:108:LYS:C   | 48:BP:110:TYR:H   | 2.05                     | 0.59              |
| 52:BT:126:ALA:C   | 52:BT:128:GLU:H   | 2.05                     | 0.59              |
| 1:AA:1306:A:H2'   | 1:AA:1307:U:H5'   | 1.84                     | 0.59              |
| 1:AA:185:A:C6     | 1:AA:186:C:C4     | 2.90                     | 0.59              |
| 1:AA:266:G:H4'    | 1:AA:267:C:H6     | 1.68                     | 0.59              |
| 1:AA:266:G:H4'    | 1:AA:267:C:C6     | 2.38                     | 0.59              |
| 1:AA:360:A:C2'    | 1:AA:361:G:C5'    | 2.80                     | 0.59              |
| 1:AA:701:C:O2'    | 1:AA:703:G:C5     | 2.50                     | 0.59              |
| 7:AG:102:ARG:O    | 7:AG:106:GLN:HB2  | 2.02                     | 0.59              |
| 9:AI:48:GLU:OE2   | 9:AI:51:ARG:HD3   | 2.03                     | 0.59              |
| 12:AL:43:VAL:HG12 | 12:AL:44:THR:N    | 2.18                     | 0.59              |
| 22:AV:39:U:H2'    | 22:AV:40:C:C6     | 2.38                     | 0.59              |
| 25:B0:10:THR:HG21 | 35:BA:2277:G:OP2  | 2.02                     | 0.59              |
| 31:B6:45:LYS:O    | 31:B6:46:HIS:HB3  | 2.02                     | 0.59              |
| 34:B9:7:VAL:HG21  | 34:B9:35:ARG:O    | 2.02                     | 0.59              |
| 35:BA:1997:G:C2'  | 35:BA:1998:G:C5'  | 2.77                     | 0.59              |
| 35:BA:2298:A:H2'  | 35:BA:2299:G:O4'  | 2.02                     | 0.59              |
| 35:BA:237:C:O2'   | 35:BA:238:C:H5'   | 2.02                     | 0.59              |
| 35:BA:860:U:C5'   | 35:BA:860:U:O2    | 2.50                     | 0.59              |
| 35:BA:890:A:C2'   | 35:BA:892:G:H5''  | 2.32                     | 0.59              |
| 38:BD:35:LYS:O    | 38:BD:37:LEU:N    | 2.35                     | 0.59              |
| 41:BG:81:LYS:HG3  | 41:BG:82:LEU:HD23 | 1.84                     | 0.59              |
| 41:BG:48:GLU:HG2  | 41:BG:87:PRO:HD2  | 1.84                     | 0.59              |
| 35:BA:1062:G:H21  | 44:BK:132:UNK:CB  | 2.15                     | 0.59              |
| 57:BY:50:ARG:HG3  | 57:BY:52:SER:O    | 2.03                     | 0.59              |
| 1:AA:956:U:C2'    | 1:AA:957:U:H5'    | 2.33                     | 0.59              |
| 7:AG:50:ILE:HD11  | 7:AG:61:VAL:CB    | 2.30                     | 0.59              |
| 14:AN:33:VAL:HA   | 14:AN:40:CYS:HA   | 1.83                     | 0.59              |
| 19:AS:5:LEU:H     | 19:AS:5:LEU:HD23  | 1.67                     | 0.59              |
| 24:AY:309:LEU:HB3 | 24:AY:391:GLY:H   | 1.66                     | 0.59              |
| 27:B2:70:GLN:CD   | 27:B2:71:ASN:H    | 2.05                     | 0.59              |
| 35:BA:108:U:O2'   | 35:BA:109:G:C5'   | 2.30                     | 0.59              |
| 35:BA:1474:C:C2'  | 35:BA:1475:G:H5'' | 2.33                     | 0.59              |
| 35:BA:1804:C:H6   | 35:BA:1804:C:O5'  | 1.85                     | 0.59              |
| 35:BA:2000:G:C2   | 35:BA:2001:A:N7   | 2.70                     | 0.59              |
| 35:BA:2379:G:H2'  | 35:BA:2380:C:C6   | 2.38                     | 0.59              |
| 35:BA:2581:G:C5   | 35:BA:2610:C:N3   | 2.70                     | 0.59              |
| 32:B7:12:ARG:HG3  | 35:BA:686:G:O6    | 2.03                     | 0.59              |
| 39:BE:117:MET:HE1 | 39:BE:136:ARG:HA  | 1.83                     | 0.59              |
| 50:BR:78:LYS:HE2  | 50:BR:83:ILE:HD11 | 1.85                     | 0.59              |
| 52:BT:128:GLU:OE1 | 52:BT:130:ALA:HB2 | 2.03                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:BY:50:ARG:C     | 57:BY:52:SER:H     | 2.06                     | 0.59              |
| 1:AA:1386:G:N2     | 1:AA:1387:G:N7     | 2.51                     | 0.59              |
| 1:AA:31:G:N1       | 1:AA:48:C:H5'      | 2.18                     | 0.59              |
| 1:AA:956:U:H2'     | 1:AA:957:U:H5'     | 1.83                     | 0.59              |
| 7:AG:74:GLU:HG2    | 7:AG:91:VAL:HG22   | 1.84                     | 0.59              |
| 22:AV:41:C:C2'     | 22:AV:42:C:C5'     | 2.79                     | 0.59              |
| 24:AY:530:VAL:HG13 | 24:AY:531:GLY:N    | 2.18                     | 0.59              |
| 25:B0:50:ASN:HB3   | 25:B0:63:VAL:HG21  | 1.83                     | 0.59              |
| 26:B1:3:LYS:CB     | 26:B1:61:ARG:NH2   | 2.65                     | 0.59              |
| 32:B7:23:ARG:HH11  | 32:B7:23:ARG:HG3   | 1.67                     | 0.59              |
| 35:BA:2202:C:H2'   | 35:BA:2203:U:H6    | 1.66                     | 0.59              |
| 35:BA:2415:G:O3'   | 48:BP:66:GLY:CA    | 2.50                     | 0.59              |
| 35:BA:613:G:C8     | 35:BA:613:G:H5'    | 2.34                     | 0.59              |
| 35:BA:674:G:H1'    | 40:BF:74:ARG:CD    | 2.32                     | 0.59              |
| 35:BA:466:A:C2     | 35:BA:796:C:O4'    | 2.55                     | 0.59              |
| 37:BC:118:PRO:C    | 37:BC:120:VAL:H    | 2.04                     | 0.59              |
| 35:BA:1568:G:O5'   | 38:BD:61:LEU:HD23  | 2.03                     | 0.59              |
| 39:BE:197:ILE:HD11 | 39:BE:199:ARG:HE   | 1.65                     | 0.59              |
| 46:BN:133:GLN:O    | 46:BN:134:ARG:HB3  | 2.02                     | 0.59              |
| 53:BU:20:LEU:HD22  | 53:BU:20:LEU:H     | 1.67                     | 0.59              |
| 53:BU:83:LEU:CD1   | 53:BU:88:ILE:HD11  | 2.33                     | 0.59              |
| 54:BV:2:PHE:CD1    | 54:BV:13:ARG:NH1   | 2.71                     | 0.59              |
| 57:BY:50:ARG:O     | 57:BY:52:SER:N     | 2.36                     | 0.59              |
| 49:BQ:63:LYS:HD2   | 58:BZ:175:VAL:HG21 | 1.85                     | 0.59              |
| 1:AA:501:C:H2'     | 1:AA:502:G:C8      | 2.38                     | 0.59              |
| 1:AA:951:G:O6      | 1:AA:1230:C:N3     | 2.36                     | 0.59              |
| 2:AB:9:GLU:N       | 2:AB:9:GLU:OE1     | 2.30                     | 0.59              |
| 4:AD:36:ARG:N      | 4:AD:37:PRO:HD3    | 2.17                     | 0.59              |
| 16:AP:45:THR:HG22  | 16:AP:47:ASP:H     | 1.66                     | 0.59              |
| 24:AY:327:PHE:CE1  | 24:AY:376:ALA:HB2  | 2.38                     | 0.59              |
| 24:AY:580:MET:O    | 24:AY:584:ILE:HG12 | 2.02                     | 0.59              |
| 26:B1:4:VAL:HA     | 26:B1:10:LYS:O     | 2.02                     | 0.59              |
| 31:B6:25:LYS:HD2   | 35:BA:2285:C:H41   | 1.66                     | 0.59              |
| 35:BA:1430:C:H6    | 35:BA:1430:C:O5'   | 1.85                     | 0.59              |
| 35:BA:1455:G:O2'   | 35:BA:1456:G:H5'   | 2.01                     | 0.59              |
| 35:BA:2000:G:C2    | 35:BA:2001:A:C5    | 2.91                     | 0.59              |
| 35:BA:824:A:O2'    | 35:BA:2358:G:O6    | 2.09                     | 0.59              |
| 35:BA:2394:C:OP1   | 48:BP:63:PRO:HD2   | 2.03                     | 0.59              |
| 35:BA:270:A:O2'    | 35:BA:271:A:H5'    | 2.03                     | 0.59              |
| 35:BA:547:A:H2'    | 35:BA:548:A:C8     | 2.37                     | 0.59              |
| 35:BA:952:G:C6     | 35:BA:966:G:C6     | 2.91                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BD:26:LYS:HA   | 38:BD:26:LYS:CE    | 2.33                     | 0.59              |
| 35:BA:2787:C:O2   | 39:BE:61:ARG:NH1   | 2.35                     | 0.59              |
| 40:BF:53:THR:HG22 | 40:BF:56:GLU:CD    | 2.24                     | 0.59              |
| 42:BH:149:ARG:HA  | 42:BH:162:ILE:HG13 | 1.85                     | 0.59              |
| 48:BP:39:LYS:HD2  | 48:BP:40:SER:H     | 1.68                     | 0.59              |
| 49:BQ:131:ILE:N   | 49:BQ:131:ILE:HD12 | 2.17                     | 0.59              |
| 57:BY:29:GLU:OE1  | 57:BY:29:GLU:N     | 2.32                     | 0.59              |
| 57:BY:52:SER:O    | 57:BY:54:LYS:N     | 2.35                     | 0.59              |
| 58:BZ:19:ARG:NH1  | 58:BZ:84:GLU:HG2   | 2.18                     | 0.59              |
| 58:BZ:5:LEU:HD21  | 58:BZ:44:PHE:HA    | 1.85                     | 0.59              |
| 1:AA:177:C:O2'    | 1:AA:178:C:H5'     | 2.02                     | 0.58              |
| 1:AA:324:G:N2     | 1:AA:327:A:OP2     | 2.37                     | 0.58              |
| 24:AY:47:GLU:HG3  | 24:AY:52:MET:SD    | 2.43                     | 0.58              |
| 26:B1:75:GLU:CA   | 26:B1:78:LYS:HD2   | 2.33                     | 0.58              |
| 29:B4:35:VAL:O    | 29:B4:36:CYS:SG    | 2.58                     | 0.58              |
| 31:B6:19:ARG:CG   | 31:B6:20:ASN:N     | 2.48                     | 0.58              |
| 33:B8:34:TRP:HA   | 35:BA:2420:C:OP1   | 2.03                     | 0.58              |
| 35:BA:1980:G:O2'  | 35:BA:1982:C:OP2   | 2.20                     | 0.58              |
| 35:BA:2406:U:O4   | 48:BP:70:GLN:HB2   | 2.03                     | 0.58              |
| 35:BA:2581:G:C5   | 35:BA:2610:C:C4    | 2.91                     | 0.58              |
| 39:BE:7:VAL:HG12  | 39:BE:27:LEU:HB3   | 1.85                     | 0.58              |
| 41:BG:53:LEU:O    | 41:BG:55:LYS:N     | 2.36                     | 0.58              |
| 41:BG:93:THR:HG22 | 41:BG:94:LEU:H     | 1.68                     | 0.58              |
| 44:BK:122:UNK:C   | 44:BK:124:UNK:N    | 2.65                     | 0.58              |
| 46:BN:133:GLN:HG2 | 46:BN:134:ARG:N    | 2.16                     | 0.58              |
| 49:BQ:141:GLN:HG3 | 58:BZ:72:ARG:NH1   | 2.18                     | 0.58              |
| 51:BS:89:ARG:CG   | 51:BS:92:TYR:HA    | 2.32                     | 0.58              |
| 1:AA:1279:A:C3'   | 1:AA:1279:A:N3     | 2.62                     | 0.58              |
| 1:AA:452:A:H1'    | 1:AA:453:A:H5''    | 1.85                     | 0.58              |
| 1:AA:89:C:O2'     | 1:AA:90:U:O5'      | 2.19                     | 0.58              |
| 1:AA:942:G:N3     | 1:AA:943:U:C5      | 2.71                     | 0.58              |
| 4:AD:150:GLU:HG2  | 4:AD:151:LYS:N     | 2.18                     | 0.58              |
| 9:AI:118:LYS:O    | 9:AI:119:ALA:HB3   | 2.02                     | 0.58              |
| 16:AP:18:ARG:CG   | 16:AP:35:LYS:HE3   | 2.32                     | 0.58              |
| 19:AS:7:LYS:O     | 19:AS:7:LYS:NZ     | 2.33                     | 0.58              |
| 1:AA:190:U:H3     | 20:AT:105:SER:CB   | 2.16                     | 0.58              |
| 24:AY:443:HIS:HB3 | 24:AY:446:THR:O    | 2.04                     | 0.58              |
| 26:B1:53:VAL:CG2  | 26:B1:58:ILE:HD12  | 2.32                     | 0.58              |
| 26:B1:6:GLU:O     | 26:B1:7:ILE:CG1    | 2.51                     | 0.58              |
| 33:B8:43:GLN:C    | 33:B8:44:LYS:HD2   | 2.23                     | 0.58              |
| 35:BA:1297:C:HO2' | 35:BA:1298:C:H5'   | 1.67                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B0:16:SER:OG    | 35:BA:2261:C:H3'   | 2.02                     | 0.58              |
| 25:B0:36:ILE:HD11  | 35:BA:2355:C:C4'   | 2.33                     | 0.58              |
| 35:BA:259:G:H2'    | 35:BA:260:G:C8     | 2.32                     | 0.58              |
| 35:BA:316:C:H2'    | 35:BA:317:G:O5'    | 2.03                     | 0.58              |
| 35:BA:528:A:H2     | 35:BA:2043:C:H5'   | 1.67                     | 0.58              |
| 41:BG:57:ALA:O     | 41:BG:61:ALA:HB2   | 2.03                     | 0.58              |
| 47:BO:20:MET:HE3   | 47:BO:44:LYS:HE3   | 1.85                     | 0.58              |
| 48:BP:97:PRO:HG3   | 48:BP:112:LEU:HD12 | 1.86                     | 0.58              |
| 54:BV:72:VAL:HG23  | 54:BV:85:LYS:HB3   | 1.84                     | 0.58              |
| 58:BZ:180:VAL:CG1  | 58:BZ:181:GLU:N    | 2.34                     | 0.58              |
| 1:AA:1078:U:H6     | 1:AA:1078:U:O5'    | 1.85                     | 0.58              |
| 1:AA:1532:U:H6     | 1:AA:1532:U:O5'    | 1.87                     | 0.58              |
| 1:AA:690:G:H8      | 1:AA:690:G:O5'     | 1.86                     | 0.58              |
| 1:AA:950:U:O2'     | 1:AA:951:G:H5''    | 2.01                     | 0.58              |
| 10:AJ:62:HIS:HB2   | 14:AN:59:ALA:HB3   | 1.85                     | 0.58              |
| 19:AS:64:GLU:O     | 29:B4:50:VAL:HG21  | 2.02                     | 0.58              |
| 20:AT:18:GLN:O     | 20:AT:22:ARG:HG3   | 2.02                     | 0.58              |
| 29:B4:30:GLU:C     | 29:B4:31:ILE:HG22  | 2.23                     | 0.58              |
| 29:B4:43:TYR:O     | 29:B4:45:GLY:N     | 2.36                     | 0.58              |
| 29:B4:61:ARG:HH11  | 29:B4:61:ARG:HB2   | 1.68                     | 0.58              |
| 34:B9:9:ARG:C      | 34:B9:10:ILE:HD12  | 2.24                     | 0.58              |
| 35:BA:1593:G:C6    | 35:BA:1594:G:C6    | 2.91                     | 0.58              |
| 35:BA:1970:A:H4'   | 35:BA:1972:A:O4'   | 2.03                     | 0.58              |
| 35:BA:2243:U:H2'   | 35:BA:2244:U:C6    | 2.39                     | 0.58              |
| 35:BA:2327:A:H2'   | 35:BA:2328:A:C8    | 2.37                     | 0.58              |
| 35:BA:296:C:O2'    | 35:BA:297:C:H5'    | 2.04                     | 0.58              |
| 40:BF:199:TRP:O    | 40:BF:203:GLN:HG2  | 2.02                     | 0.58              |
| 41:BG:112:PRO:O    | 41:BG:113:ARG:HB3  | 2.03                     | 0.58              |
| 41:BG:172:LEU:HD23 | 41:BG:172:LEU:O    | 2.03                     | 0.58              |
| 46:BN:4:TYR:HB3    | 53:BU:64:ARG:NH1   | 2.04                     | 0.58              |
| 47:BO:9:GLU:HG3    | 47:BO:18:LYS:NZ    | 2.19                     | 0.58              |
| 50:BR:55:ALA:HB2   | 50:BR:79:LEU:CD1   | 2.32                     | 0.58              |
| 51:BS:28:VAL:HB    | 51:BS:89:ARG:HB2   | 1.86                     | 0.58              |
| 51:BS:34:HIS:CB    | 51:BS:53:SER:HB3   | 2.32                     | 0.58              |
| 1:AA:204:U:O4'     | 1:AA:216:G:C8      | 2.57                     | 0.58              |
| 1:AA:555:C:N4      | 1:AA:556:C:N4      | 2.51                     | 0.58              |
| 1:AA:594:G:O2'     | 1:AA:595:G:H5'     | 2.04                     | 0.58              |
| 1:AA:940:C:O5'     | 1:AA:940:C:H6      | 1.85                     | 0.58              |
| 7:AG:76:ARG:HD2    | 7:AG:156:TRP:CZ2   | 2.39                     | 0.58              |
| 7:AG:70:LYS:HD3    | 7:AG:96:GLN:HB3    | 1.85                     | 0.58              |
| 9:AI:95:LYS:HZ2    | 9:AI:96:LEU:HD13   | 1.67                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:600:VAL:CG2  | 24:AY:678:GLU:HG3  | 2.34                     | 0.58              |
| 29:B4:13:ARG:N     | 29:B4:24:THR:CG2   | 2.64                     | 0.58              |
| 29:B4:56:VAL:CG2   | 29:B4:60:GLN:HG3   | 2.33                     | 0.58              |
| 33:B8:61:LEU:N     | 33:B8:61:LEU:HD12  | 2.18                     | 0.58              |
| 35:BA:1048:A:N6    | 42:BH:1:MET:CE     | 2.67                     | 0.58              |
| 35:BA:18:C:H2'     | 35:BA:19:C:C5      | 2.37                     | 0.58              |
| 35:BA:47:C:C4      | 35:BA:179:G:N1     | 2.71                     | 0.58              |
| 35:BA:692:C:C2'    | 35:BA:693:C:C5'    | 2.77                     | 0.58              |
| 39:BE:13:ARG:O     | 52:BT:57:PHE:HE2   | 1.86                     | 0.58              |
| 35:BA:2784:C:H1'   | 39:BE:37:ARG:HH12  | 1.68                     | 0.58              |
| 40:BF:185:ASP:HA   | 40:BF:188:ARG:HG2  | 1.84                     | 0.58              |
| 41:BG:6:ALA:HB3    | 41:BG:105:LYS:CE   | 2.33                     | 0.58              |
| 48:BP:16:ARG:O     | 48:BP:16:ARG:NH1   | 2.35                     | 0.58              |
| 53:BU:76:TYR:OH    | 53:BU:93:LYS:HE3   | 2.03                     | 0.58              |
| 1:AA:1154:G:HO2'   | 1:AA:1155:G:H5'    | 1.66                     | 0.58              |
| 1:AA:1163:C:H2'    | 1:AA:1164:G:H8     | 1.67                     | 0.58              |
| 1:AA:1296:C:H4'    | 1:AA:1302:U:C4     | 2.38                     | 0.58              |
| 1:AA:1391:U:H2'    | 1:AA:1392:G:H8     | 1.66                     | 0.58              |
| 10:AJ:74:ILE:HG13  | 10:AJ:74:ILE:O     | 2.03                     | 0.58              |
| 15:AO:39:LEU:HB3   | 15:AO:56:LEU:HD23  | 1.85                     | 0.58              |
| 24:AY:15:ILE:HG22  | 24:AY:103:GLY:C    | 2.24                     | 0.58              |
| 27:B2:9:GLN:O      | 27:B2:11:GLU:N     | 2.37                     | 0.58              |
| 34:B9:32:HIS:O     | 34:B9:34:GLN:HG3   | 2.03                     | 0.58              |
| 35:BA:1778:U:C2'   | 35:BA:1779:U:H5'   | 2.32                     | 0.58              |
| 35:BA:1999:C:H2'   | 35:BA:2000:G:H8    | 1.68                     | 0.58              |
| 35:BA:2523:G:C2'   | 35:BA:2524:G:H5''  | 2.32                     | 0.58              |
| 49:BQ:141:GLN:N    | 58:BZ:53:ILE:HD12  | 2.18                     | 0.58              |
| 53:BU:74:LEU:HD11  | 53:BU:79:PHE:HB2   | 1.85                     | 0.58              |
| 58:BZ:51:ALA:HB1   | 58:BZ:57:ILE:CD1   | 2.32                     | 0.58              |
| 1:AA:1071:C:H2'    | 1:AA:1072:G:H8     | 1.67                     | 0.58              |
| 1:AA:1306:A:N6     | 1:AA:1331:G:O2'    | 2.36                     | 0.58              |
| 1:AA:840:C:H5'     | 1:AA:841:U:OP1     | 2.02                     | 0.58              |
| 2:AB:122:PHE:CE2   | 2:AB:142:LEU:CD2   | 2.79                     | 0.58              |
| 2:AB:167:PRO:HD2   | 2:AB:188:ALA:CB    | 2.26                     | 0.58              |
| 2:AB:166:ASP:OD2   | 2:AB:169:LYS:HB2   | 2.03                     | 0.58              |
| 8:AH:122:ARG:NH1   | 8:AH:122:ARG:HB2   | 2.18                     | 0.58              |
| 14:AN:32:SER:HB3   | 14:AN:41:ARG:HG3   | 1.84                     | 0.58              |
| 24:AY:137:ASN:HD21 | 24:AY:263:ALA:H    | 1.51                     | 0.58              |
| 24:AY:517:LEU:N    | 24:AY:517:LEU:HD12 | 2.18                     | 0.58              |
| 25:B0:50:ASN:O     | 25:B0:62:LEU:CD2   | 2.52                     | 0.58              |
| 26:B1:11:ARG:HG2   | 26:B1:11:ARG:NH1   | 2.17                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:B1:6:GLU:O      | 26:B1:7:ILE:HG12   | 2.03                     | 0.58              |
| 33:B8:41:ILE:HD12  | 35:BA:2419:U:OP1   | 2.03                     | 0.58              |
| 35:BA:184:C:H2'    | 35:BA:185:U:C6     | 2.38                     | 0.58              |
| 35:BA:1676:A:H2    | 35:BA:1993:U:H5'   | 1.66                     | 0.58              |
| 35:BA:2150:U:H2'   | 35:BA:2151:G:H8    | 1.68                     | 0.58              |
| 35:BA:272(C):G:H2' | 35:BA:272(D):G:H8  | 1.69                     | 0.58              |
| 35:BA:554:U:O2'    | 35:BA:555:U:H5'    | 2.04                     | 0.58              |
| 37:BC:73:VAL:HG13  | 37:BC:74:ARG:H     | 1.67                     | 0.58              |
| 39:BE:132:HIS:CG   | 39:BE:135:HIS:CE1  | 2.92                     | 0.58              |
| 42:BH:88:LEU:HD23  | 42:BH:164:TYR:O    | 2.04                     | 0.58              |
| 42:BH:46:GLU:OE2   | 42:BH:51:ARG:HD2   | 2.04                     | 0.58              |
| 46:BN:63:THR:O     | 46:BN:66:LYS:HG3   | 2.04                     | 0.58              |
| 48:BP:139:LYS:O    | 48:BP:141:ALA:N    | 2.30                     | 0.58              |
| 51:BS:101:LEU:O    | 51:BS:101:LEU:HD12 | 2.04                     | 0.58              |
| 54:BV:25:LEU:N     | 54:BV:92:THR:HG21  | 2.17                     | 0.58              |
| 1:AA:1029:C:N4     | 1:AA:1033:G:H1     | 2.01                     | 0.58              |
| 1:AA:1221:G:O2'    | 1:AA:1222:G:H5'    | 2.02                     | 0.58              |
| 1:AA:1388:C:O2'    | 1:AA:1389:C:C5'    | 2.50                     | 0.58              |
| 1:AA:954:G:H2'     | 1:AA:955:U:C6      | 2.39                     | 0.58              |
| 1:AA:962:C:H2'     | 1:AA:963:G:H8      | 1.66                     | 0.58              |
| 3:AC:167:TRP:NE1   | 3:AC:168:ALA:O     | 2.37                     | 0.58              |
| 4:AD:70:ILE:HG22   | 4:AD:71:SER:O      | 2.03                     | 0.58              |
| 8:AH:1:MET:HE3     | 8:AH:1:MET:H3      | 1.68                     | 0.58              |
| 11:AK:84:VAL:HG11  | 11:AK:91:ARG:HD3   | 1.84                     | 0.58              |
| 1:AA:502:G:OP1     | 12:AL:118:SER:HB3  | 2.03                     | 0.58              |
| 19:AS:40:ILE:HG23  | 19:AS:67:VAL:O     | 2.02                     | 0.58              |
| 21:AU:12:LYS:HB3   | 21:AU:22:ARG:HD2   | 1.85                     | 0.58              |
| 25:B0:11:ARG:O     | 25:B0:13:GLY:N     | 2.31                     | 0.58              |
| 25:B0:53:MET:HE1   | 25:B0:57:PHE:HD2   | 1.68                     | 0.58              |
| 25:B0:46:LYS:CE    | 25:B0:75:LEU:O     | 2.52                     | 0.58              |
| 26:B1:4:VAL:HG23   | 26:B1:10:LYS:O     | 2.03                     | 0.58              |
| 35:BA:1516:C:O2'   | 35:BA:1517:G:H5''  | 2.04                     | 0.58              |
| 35:BA:1701:A:C3'   | 35:BA:1702:G:H5'   | 2.34                     | 0.58              |
| 35:BA:1798:U:O2    | 35:BA:1821:A:H2    | 1.87                     | 0.58              |
| 35:BA:271(L):U:H4' | 35:BA:271(M):G:C8  | 2.38                     | 0.58              |
| 35:BA:272(J):C:H2' | 35:BA:274:G:C5'    | 2.34                     | 0.58              |
| 35:BA:527:C:H1'    | 35:BA:528:A:N7     | 2.18                     | 0.58              |
| 35:BA:654(O):G:H2' | 35:BA:654(P):C:C6  | 2.38                     | 0.58              |
| 35:BA:747:U:C5     | 35:BA:2613:U:N3    | 2.72                     | 0.58              |
| 1:AA:682:G:C5'     | 38:BD:169:GLU:OE1  | 2.52                     | 0.58              |
| 41:BG:141:PHE:CD1  | 41:BG:142:PRO:HA   | 2.30                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:536:C:H2'    | 1:AA:537:G:C8      | 2.39                     | 0.58              |
| 1:AA:796:C:C2'    | 1:AA:797:C:H5'     | 2.34                     | 0.58              |
| 3:AC:46:GLU:OE1   | 3:AC:83:ARG:NH2    | 2.37                     | 0.58              |
| 7:AG:88:PRO:O     | 7:AG:89:MET:CB     | 2.51                     | 0.58              |
| 25:B0:66:VAL:O    | 25:B0:81:VAL:CG1   | 2.51                     | 0.58              |
| 35:BA:1914:C:H5'  | 35:BA:1915:U:OP2   | 2.04                     | 0.58              |
| 35:BA:2145:C:H5'  | 35:BA:2146:C:H5    | 1.66                     | 0.58              |
| 35:BA:2710:C:C2'  | 35:BA:2711:A:H5'   | 2.33                     | 0.58              |
| 35:BA:407:G:H2'   | 35:BA:408:G:C8     | 2.37                     | 0.58              |
| 39:BE:25:VAL:CG1  | 39:BE:181:LEU:HD12 | 2.33                     | 0.58              |
| 39:BE:47:VAL:O    | 39:BE:49:LEU:HD23  | 2.04                     | 0.58              |
| 40:BF:24:LEU:CB   | 40:BF:25:PRO:HD2   | 2.30                     | 0.58              |
| 41:BG:73:ALA:HB3  | 41:BG:85:GLY:HA2   | 1.85                     | 0.58              |
| 46:BN:126:PRO:O   | 46:BN:127:ASP:O    | 2.21                     | 0.58              |
| 46:BN:57:ALA:C    | 46:BN:58:ASP:O     | 2.41                     | 0.58              |
| 52:BT:35:LYS:CE   | 52:BT:41:ARG:HD2   | 2.34                     | 0.58              |
| 57:BY:44:ILE:H    | 57:BY:44:ILE:HD12  | 1.68                     | 0.58              |
| 58:BZ:67:LEU:HD12 | 58:BZ:67:LEU:O     | 2.04                     | 0.58              |
| 1:AA:1154:G:H2'   | 1:AA:1155:G:H8     | 1.69                     | 0.58              |
| 1:AA:874:G:C4     | 1:AA:875:C:C5      | 2.92                     | 0.58              |
| 3:AC:22:TRP:O     | 3:AC:22:TRP:CD2    | 2.56                     | 0.58              |
| 11:AK:92:GLU:HG3  | 11:AK:96:ARG:NH2   | 2.18                     | 0.58              |
| 17:AQ:63:ARG:O    | 17:AQ:65:ILE:HD12  | 2.03                     | 0.58              |
| 24:AY:156:ARG:NH2 | 24:AY:666:ARG:CZ   | 2.67                     | 0.58              |
| 24:AY:478:LYS:HA  | 24:AY:653:PHE:CE1  | 2.38                     | 0.58              |
| 29:B4:53:GLU:CD   | 29:B4:54:GLY:N     | 2.57                     | 0.58              |
| 31:B6:51:GLU:O    | 31:B6:52:VAL:HB    | 2.04                     | 0.58              |
| 35:BA:1299:G:H8   | 35:BA:1299:G:O5'   | 1.86                     | 0.58              |
| 35:BA:1422:G:H2'  | 35:BA:1423:G:H8    | 1.69                     | 0.58              |
| 35:BA:15:G:H2'    | 35:BA:16:G:H8      | 1.69                     | 0.58              |
| 35:BA:2124:G:H2'  | 35:BA:2125:G:H5'   | 1.86                     | 0.58              |
| 35:BA:2754:U:O5'  | 35:BA:2754:U:H6    | 1.86                     | 0.58              |
| 35:BA:2836:U:H2'  | 35:BA:2837:G:H8    | 1.65                     | 0.58              |
| 35:BA:600:G:C2'   | 35:BA:601:C:H5'    | 2.34                     | 0.58              |
| 37:BC:108:TRP:C   | 37:BC:110:ASP:H    | 2.07                     | 0.58              |
| 47:BO:10:VAL:HG21 | 47:BO:16:ALA:C     | 2.24                     | 0.58              |
| 50:BR:58:GLY:HA2  | 50:BR:80:PHE:HE2   | 1.69                     | 0.58              |
| 56:BX:35:THR:O    | 56:BX:39:ILE:HG13  | 2.04                     | 0.58              |
| 58:BZ:10:ARG:NH2  | 58:BZ:26:GLY:O     | 2.36                     | 0.58              |
| 35:BA:1076:C:H4'  | 58:BZ:112:ARG:NH2  | 2.17                     | 0.58              |
| 58:BZ:48:PHE:CE1  | 58:BZ:52:SER:HA    | 2.39                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1049:U:C2'   | 14:AN:2:ALA:N      | 2.67                     | 0.58              |
| 1:AA:1316:G:N2    | 1:AA:1318:A:H3'    | 2.19                     | 0.58              |
| 2:AB:12:GLU:O     | 2:AB:16:HIS:HB2    | 2.04                     | 0.58              |
| 3:AC:19:GLU:O     | 3:AC:56:ASP:HA     | 2.03                     | 0.58              |
| 3:AC:35:GLU:HG2   | 3:AC:39:ILE:CD1    | 2.34                     | 0.58              |
| 3:AC:53:ALA:O     | 3:AC:54:ARG:CB     | 2.51                     | 0.58              |
| 8:AH:83:ILE:HG23  | 8:AH:83:ILE:O      | 2.04                     | 0.58              |
| 1:AA:1118:C:OP1   | 9:AI:104:ARG:NH1   | 2.37                     | 0.58              |
| 9:AI:121:ARG:HH11 | 9:AI:121:ARG:HG2   | 1.68                     | 0.58              |
| 13:AM:40:ASN:ND2  | 13:AM:43:THR:HG23  | 2.19                     | 0.58              |
| 19:AS:86:GLU:O    | 19:AS:87:ALA:HB3   | 2.03                     | 0.58              |
| 24:AY:104:ALA:C   | 24:AY:105:ILE:HD12 | 2.24                     | 0.58              |
| 24:AY:488:THR:OG1 | 24:AY:598:ASP:HB3  | 2.04                     | 0.58              |
| 32:B7:12:ARG:CD   | 32:B7:46:VAL:HG21  | 2.34                     | 0.58              |
| 35:BA:1027:A:C6   | 35:BA:1126:A:C4    | 2.92                     | 0.58              |
| 35:BA:107:C:O2'   | 35:BA:108:U:H5'    | 2.03                     | 0.58              |
| 35:BA:1463:C:O2'  | 35:BA:1464:C:H5'   | 2.03                     | 0.58              |
| 35:BA:1652:A:N6   | 35:BA:1653:G:H1    | 2.00                     | 0.58              |
| 35:BA:752:A:C5    | 35:BA:1781:C:O4'   | 2.57                     | 0.58              |
| 35:BA:2199:A:C5'  | 35:BA:2200:C:OP2   | 2.52                     | 0.58              |
| 35:BA:857:C:N4    | 35:BA:858:U:O4     | 2.36                     | 0.58              |
| 35:BA:1798:U:C5   | 38:BD:274:ARG:NH2  | 2.71                     | 0.58              |
| 38:BD:35:LYS:HZ2  | 38:BD:35:LYS:CB    | 2.15                     | 0.58              |
| 39:BE:9:VAL:HG13  | 39:BE:25:VAL:HB    | 1.86                     | 0.58              |
| 46:BN:10:GLU:OE2  | 46:BN:11:PRO:HD2   | 2.03                     | 0.58              |
| 35:BA:195:A:H5''  | 48:BP:46:LYS:NZ    | 2.18                     | 0.58              |
| 51:BS:35:ILE:H    | 51:BS:53:SER:CB    | 2.08                     | 0.58              |
| 53:BU:65:ILE:HD11 | 53:BU:96:ALA:HB3   | 1.85                     | 0.58              |
| 57:BY:3:VAL:H     | 57:BY:5:MET:HE3    | 1.68                     | 0.58              |
| 58:BZ:48:PHE:CE2  | 58:BZ:74:VAL:HG21  | 2.28                     | 0.58              |
| 1:AA:1414:U:H2'   | 1:AA:1415:G:H8     | 1.69                     | 0.57              |
| 10:AJ:51:ARG:HG3  | 10:AJ:60:ARG:HA    | 1.85                     | 0.57              |
| 19:AS:7:LYS:HD3   | 19:AS:7:LYS:N      | 2.19                     | 0.57              |
| 24:AY:343:ASN:C   | 24:AY:343:ASN:HD22 | 2.06                     | 0.57              |
| 24:AY:379:GLY:O   | 24:AY:380:LEU:HB2  | 2.03                     | 0.57              |
| 24:AY:496:LYS:HE2 | 24:AY:498:ILE:HD13 | 1.85                     | 0.57              |
| 24:AY:57:GLN:O    | 24:AY:58:GLU:C     | 2.42                     | 0.57              |
| 27:B2:64:LEU:CD2  | 27:B2:64:LEU:C     | 2.72                     | 0.57              |
| 30:B5:16:ARG:NH1  | 30:B5:16:ARG:HG2   | 2.17                     | 0.57              |
| 31:B6:40:CYS:SG   | 31:B6:45:LYS:NZ    | 2.71                     | 0.57              |
| 35:BA:1458:C:H5'  | 35:BA:1459:G:C8    | 2.39                     | 0.57              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 35:BA:1484:G:C3'    | 35:BA:1485:G:H5'' | 2.34                     | 0.57              |
| 35:BA:1528(A):A:H62 | 35:BA:1541:G:H21  | 1.50                     | 0.57              |
| 35:BA:272(J):C:H2'  | 35:BA:274:G:H5'   | 1.84                     | 0.57              |
| 35:BA:300:A:H2'     | 35:BA:334:C:H1'   | 1.86                     | 0.57              |
| 36:BB:25:A:H3'      | 36:BB:26:A:H8     | 1.69                     | 0.57              |
| 36:BB:56:G:O2'      | 36:BB:57:A:OP2    | 2.22                     | 0.57              |
| 37:BC:103:LYS:O     | 37:BC:103:LYS:HG3 | 2.03                     | 0.57              |
| 37:BC:103:LYS:O     | 37:BC:105:LEU:N   | 2.36                     | 0.57              |
| 42:BH:3:ARG:CG      | 42:BH:3:ARG:NH1   | 2.63                     | 0.57              |
| 48:BP:79:ARG:H      | 48:BP:110:TYR:HD2 | 1.52                     | 0.57              |
| 50:BR:87:TYR:C      | 50:BR:89:ASP:H    | 2.07                     | 0.57              |
| 51:BS:35:ILE:HG23   | 51:BS:35:ILE:O    | 2.03                     | 0.57              |
| 52:BT:81:PRO:O      | 52:BT:82:LEU:HG   | 2.04                     | 0.57              |
| 58:BZ:97:GLU:HA     | 58:BZ:127:LYS:HA  | 1.85                     | 0.57              |
| 1:AA:109:A:H3'      | 1:AA:110:C:H5'    | 1.85                     | 0.57              |
| 1:AA:563:A:H3'      | 1:AA:563:A:N3     | 2.19                     | 0.57              |
| 1:AA:651:C:O2'      | 1:AA:652:U:H5'    | 2.04                     | 0.57              |
| 1:AA:723:U:H2'      | 1:AA:723:U:O2     | 2.04                     | 0.57              |
| 1:AA:757:U:H2'      | 1:AA:758:G:O4'    | 2.04                     | 0.57              |
| 1:AA:919:A:O5'      | 1:AA:919:A:H8     | 1.87                     | 0.57              |
| 9:AI:95:LYS:HD2     | 9:AI:95:LYS:C     | 2.25                     | 0.57              |
| 17:AQ:67:LYS:O      | 17:AQ:68:ARG:CB   | 2.53                     | 0.57              |
| 24:AY:55:MET:HG3    | 24:AY:56:GLU:H    | 1.66                     | 0.57              |
| 25:B0:80:HIS:H      | 25:B0:80:HIS:CD2  | 2.21                     | 0.57              |
| 26:B1:40:ARG:HH11   | 26:B1:40:ARG:HG2  | 1.69                     | 0.57              |
| 28:B3:45:GLY:HA3    | 35:BA:851:U:O2'   | 2.04                     | 0.57              |
| 31:B6:20:ASN:O      | 31:B6:21:TYR:CG   | 2.57                     | 0.57              |
| 33:B8:63:PRO:O      | 33:B8:64:TYR:O    | 2.22                     | 0.57              |
| 35:BA:1462:C:H2'    | 35:BA:1463:C:C6   | 2.39                     | 0.57              |
| 35:BA:1607:C:H4'    | 35:BA:1608:A:O5'  | 2.03                     | 0.57              |
| 35:BA:1914:C:H5''   | 35:BA:1915:U:H5   | 1.68                     | 0.57              |
| 35:BA:2029:G:N1     | 35:BA:2033:A:OP1  | 2.37                     | 0.57              |
| 35:BA:332:A:OP2     | 35:BA:332:A:H3'   | 2.03                     | 0.57              |
| 35:BA:461:C:O5'     | 35:BA:461:C:H6    | 1.86                     | 0.57              |
| 35:BA:588:U:H2'     | 35:BA:589:C:C6    | 2.39                     | 0.57              |
| 35:BA:621:A:H2'     | 35:BA:622:G:H5'   | 1.85                     | 0.57              |
| 35:BA:651:G:H2'     | 35:BA:652:C:H5'   | 1.85                     | 0.57              |
| 35:BA:697:C:C2'     | 35:BA:698:C:C5'   | 2.78                     | 0.57              |
| 37:BC:6:LYS:HG3     | 37:BC:7:ARG:H     | 1.69                     | 0.57              |
| 38:BD:24:ILE:CG2    | 38:BD:25:THR:N    | 2.59                     | 0.57              |
| 38:BD:2:ALA:O       | 38:BD:3:VAL:HG23  | 2.04                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:48:GLU:O     | 41:BG:49:ASP:HB2   | 2.05                     | 0.57              |
| 41:BG:5:VAL:CG1    | 41:BG:8:LYS:HB2    | 2.34                     | 0.57              |
| 41:BG:9:ARG:HD2    | 41:BG:9:ARG:H      | 1.69                     | 0.57              |
| 52:BT:125:ARG:HG2  | 52:BT:125:ARG:HH11 | 1.69                     | 0.57              |
| 52:BT:25:GLY:O     | 52:BT:48:ILE:HG23  | 2.05                     | 0.57              |
| 52:BT:46:GLU:HB3   | 52:BT:65:LYS:HE3   | 1.85                     | 0.57              |
| 56:BX:26:TYR:OH    | 56:BX:88:LYS:HD2   | 2.04                     | 0.57              |
| 1:AA:180:U:H2'     | 1:AA:181:G:H5'     | 1.86                     | 0.57              |
| 1:AA:952:U:C2'     | 1:AA:953:G:H5'     | 2.34                     | 0.57              |
| 2:AB:87:ARG:CD     | 2:AB:219:VAL:CG1   | 2.82                     | 0.57              |
| 3:AC:191:THR:HG22  | 3:AC:192:THR:H     | 1.69                     | 0.57              |
| 20:AT:37:SER:O     | 20:AT:41:ILE:HG12  | 2.03                     | 0.57              |
| 24:AY:385:THR:HG21 | 24:AY:436:PRO:HD3  | 1.86                     | 0.57              |
| 24:AY:57:GLN:O     | 24:AY:60:GLU:HB2   | 2.03                     | 0.57              |
| 24:AY:57:GLN:O     | 24:AY:60:GLU:CB    | 2.53                     | 0.57              |
| 29:B4:17:GLY:H     | 29:B4:33:VAL:HG11  | 1.69                     | 0.57              |
| 31:B6:9:LEU:CD1    | 31:B6:11:LEU:HD12  | 2.34                     | 0.57              |
| 34:B9:27:CYS:SG    | 34:B9:28:GLU:N     | 2.76                     | 0.57              |
| 35:BA:1060:U:C5    | 35:BA:1062:G:H4'   | 2.39                     | 0.57              |
| 35:BA:2267:A:H5''  | 35:BA:2268:A:H5'   | 1.86                     | 0.57              |
| 35:BA:2715:C:C2    | 35:BA:2716:U:C5    | 2.91                     | 0.57              |
| 35:BA:604:G:C6     | 35:BA:605:C:N4     | 2.73                     | 0.57              |
| 36:BB:45:A:H1'     | 41:BG:95:ARG:NH2   | 2.19                     | 0.57              |
| 46:BN:22:THR:HA    | 46:BN:61:ARG:O     | 2.05                     | 0.57              |
| 1:AA:1000:U:H2'    | 1:AA:1001:A:C8     | 2.39                     | 0.57              |
| 1:AA:1251:A:H2'    | 1:AA:1252:A:C8     | 2.39                     | 0.57              |
| 1:AA:1468:A:H2'    | 1:AA:1469:G:O4'    | 2.04                     | 0.57              |
| 1:AA:942:G:C6      | 1:AA:943:U:C4      | 2.92                     | 0.57              |
| 2:AB:168:THR:CG2   | 2:AB:192:SER:HA    | 2.34                     | 0.57              |
| 8:AH:33:GLU:OE1    | 8:AH:50:ARG:NH1    | 2.37                     | 0.57              |
| 1:AA:1203:C:OP1    | 14:AN:3:ARG:HD2    | 2.04                     | 0.57              |
| 1:AA:1216:G:H5''   | 14:AN:5:ALA:CB     | 2.33                     | 0.57              |
| 24:AY:600:VAL:HG21 | 24:AY:678:GLU:HG3  | 1.86                     | 0.57              |
| 35:BA:1038:C:H3'   | 35:BA:1039:G:C5'   | 2.20                     | 0.57              |
| 35:BA:1464:C:H1'   | 35:BA:1528:A:H8    | 1.69                     | 0.57              |
| 35:BA:1891:G:H2'   | 35:BA:1892:C:C6    | 2.40                     | 0.57              |
| 35:BA:272(I):U:C5' | 35:BA:272(I):U:H6  | 2.16                     | 0.57              |
| 35:BA:2748:A:C4    | 35:BA:2757:A:C6    | 2.92                     | 0.57              |
| 35:BA:654(A):G:O2' | 35:BA:654(B):C:H5' | 2.05                     | 0.57              |
| 37:BC:117:THR:N    | 37:BC:118:PRO:CA   | 2.35                     | 0.57              |
| 42:BH:19:VAL:O     | 42:BH:20:ALA:HB3   | 2.03                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:BH:7:LEU:CD2    | 42:BH:69:ARG:HE   | 2.16                     | 0.57              |
| 35:BA:826:U:O2'    | 48:BP:54:GLY:HA3  | 2.03                     | 0.57              |
| 54:BV:47:VAL:HG23  | 54:BV:47:VAL:O    | 2.03                     | 0.57              |
| 56:BX:50:LYS:H     | 56:BX:87:GLN:HE22 | 1.52                     | 0.57              |
| 1:AA:1054:C:OP1    | 1:AA:1197:G:OP1   | 2.22                     | 0.57              |
| 1:AA:1237:C:HO2'   | 1:AA:1335:C:C1'   | 2.12                     | 0.57              |
| 1:AA:1302:U:C5     | 13:AM:17:VAL:HG21 | 2.39                     | 0.57              |
| 1:AA:324:G:H22     | 1:AA:327:A:P      | 2.27                     | 0.57              |
| 1:AA:488:C:O2'     | 1:AA:489:C:H5'    | 2.05                     | 0.57              |
| 1:AA:832:C:O2'     | 1:AA:833:U:H5'    | 2.05                     | 0.57              |
| 2:AB:97:TRP:HZ3    | 2:AB:176:GLU:OE2  | 1.86                     | 0.57              |
| 2:AB:75:LYS:O      | 2:AB:77:ALA:N     | 2.37                     | 0.57              |
| 3:AC:72:LYS:HE3    | 3:AC:74:GLY:HA3   | 1.86                     | 0.57              |
| 4:AD:116:GLN:NE2   | 4:AD:157:LEU:HD21 | 2.19                     | 0.57              |
| 5:AE:11:ILE:HD11   | 5:AE:31:LEU:HD22  | 1.86                     | 0.57              |
| 10:AJ:22:LYS:NZ    | 10:AJ:90:LEU:HD22 | 2.19                     | 0.57              |
| 16:AP:8:ARG:HB3    | 16:AP:28:ARG:NH1  | 2.19                     | 0.57              |
| 24:AY:232:LEU:HD13 | 24:AY:232:LEU:N   | 2.20                     | 0.57              |
| 24:AY:137:ASN:ND2  | 24:AY:263:ALA:H   | 2.03                     | 0.57              |
| 24:AY:517:LEU:HD11 | 24:AY:564:LYS:HB2 | 1.85                     | 0.57              |
| 25:B0:14:ARG:CG    | 25:B0:14:ARG:NH1  | 2.63                     | 0.57              |
| 30:B5:3:LYS:HA     | 30:B5:3:LYS:HE3   | 1.86                     | 0.57              |
| 35:BA:1068:G:N3    | 35:BA:1068:G:H2'  | 2.19                     | 0.57              |
| 35:BA:1422:G:C5    | 35:BA:1423:G:N7   | 2.72                     | 0.57              |
| 35:BA:16:G:H2'     | 35:BA:17:G:H8     | 1.69                     | 0.57              |
| 35:BA:1864:U:C3'   | 35:BA:1865:G:H5'' | 2.34                     | 0.57              |
| 35:BA:221:A:N6     | 35:BA:265:A:H8    | 2.03                     | 0.57              |
| 35:BA:8:A:H2'      | 35:BA:9:U:C6      | 2.40                     | 0.57              |
| 38:BD:142:VAL:HG21 | 38:BD:191:ALA:HB1 | 1.87                     | 0.57              |
| 39:BE:77:ILE:HG22  | 39:BE:78:LEU:N    | 2.09                     | 0.57              |
| 40:BF:63:LYS:HA    | 40:BF:76:GLY:O    | 2.04                     | 0.57              |
| 41:BG:147:ASP:O    | 41:BG:148:MET:C   | 2.42                     | 0.57              |
| 42:BH:20:ALA:HB1   | 42:BH:21:PRO:HD2  | 1.85                     | 0.57              |
| 44:BK:57:UNK:HA    | 44:BK:67:UNK:CA   | 2.34                     | 0.57              |
| 57:BY:95:LYS:HD2   | 57:BY:100:ALA:CA  | 2.34                     | 0.57              |
| 58:BZ:122:ARG:HB3  | 58:BZ:122:ARG:NH1 | 2.19                     | 0.57              |
| 1:AA:119:A:O2'     | 1:AA:120:A:P      | 2.62                     | 0.57              |
| 1:AA:872:A:O2'     | 1:AA:873:A:H3'    | 2.04                     | 0.57              |
| 2:AB:71:VAL:HB     | 2:AB:164:VAL:HG22 | 1.85                     | 0.57              |
| 3:AC:86:VAL:CG2    | 3:AC:87:LEU:N     | 2.68                     | 0.57              |
| 7:AG:88:PRO:HG2    | 7:AG:152:ALA:HB2  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AT:100:ILE:O   | 20:AT:101:GLY:C    | 2.42                     | 0.57              |
| 27:B2:17:SER:CB   | 27:B2:18:PRO:HD2   | 2.34                     | 0.57              |
| 29:B4:33:VAL:HG22 | 29:B4:34:GLU:H     | 1.69                     | 0.57              |
| 33:B8:61:LEU:CD1  | 33:B8:63:PRO:HD2   | 2.34                     | 0.57              |
| 35:BA:1022:G:N2   | 35:BA:1142(A):A:H2 | 1.99                     | 0.57              |
| 35:BA:1701:A:C2'  | 35:BA:1702:G:H5'   | 2.34                     | 0.57              |
| 35:BA:1769:G:H2'  | 35:BA:1770:G:H5'   | 1.84                     | 0.57              |
| 35:BA:309:G:N3    | 35:BA:329:G:O2'    | 2.37                     | 0.57              |
| 39:BE:56:PRO:O    | 39:BE:57:LYS:CE    | 2.53                     | 0.57              |
| 41:BG:122:PRO:HD3 | 41:BG:181:ARG:HA   | 1.87                     | 0.57              |
| 41:BG:122:PRO:O   | 41:BG:124:SER:N    | 2.37                     | 0.57              |
| 41:BG:85:GLY:O    | 41:BG:86:MET:CB    | 2.51                     | 0.57              |
| 46:BN:34:LEU:HD21 | 46:BN:120:LEU:HB2  | 1.87                     | 0.57              |
| 50:BR:52:ILE:O    | 50:BR:55:ALA:HB3   | 2.04                     | 0.57              |
| 1:AA:1435:G:H2'   | 1:AA:1436:U:C6     | 2.38                     | 0.57              |
| 1:AA:35:G:H2'     | 1:AA:36:C:C6       | 2.39                     | 0.57              |
| 1:AA:573:A:H5'    | 1:AA:573:A:C8      | 2.38                     | 0.57              |
| 1:AA:593:G:H2'    | 1:AA:594:G:C5'     | 2.32                     | 0.57              |
| 2:AB:91:PRO:HA    | 2:AB:151:GLY:O     | 2.05                     | 0.57              |
| 3:AC:103:VAL:HG12 | 3:AC:104:GLN:N     | 2.20                     | 0.57              |
| 5:AE:64:ARG:O     | 5:AE:64:ARG:HG2    | 2.05                     | 0.57              |
| 10:AJ:58:ASP:O    | 10:AJ:59:SER:CB    | 2.49                     | 0.57              |
| 18:AR:26:LEU:HD21 | 18:AR:42:ARG:HH22  | 1.67                     | 0.57              |
| 19:AS:67:VAL:HB   | 29:B4:50:VAL:CG1   | 2.34                     | 0.57              |
| 1:AA:1313:U:C6    | 19:AS:6:LYS:NZ     | 2.73                     | 0.57              |
| 20:AT:84:LEU:O    | 20:AT:88:VAL:HG23  | 2.05                     | 0.57              |
| 24:AY:9:LEU:HD21  | 24:AY:284:LEU:HD13 | 1.86                     | 0.57              |
| 29:B4:21:VAL:CG2  | 29:B4:35:VAL:CG2   | 2.83                     | 0.57              |
| 33:B8:54:GLU:O    | 33:B8:58:ILE:HG12  | 2.04                     | 0.57              |
| 35:BA:1054:A:O2'  | 35:BA:1055:G:H5'   | 2.05                     | 0.57              |
| 35:BA:1906:G:H2'  | 35:BA:1907:G:O4'   | 2.05                     | 0.57              |
| 35:BA:1970:A:C4'  | 35:BA:1972:A:O4'   | 2.52                     | 0.57              |
| 35:BA:2340:G:O2'  | 35:BA:2341:G:H5'   | 2.05                     | 0.57              |
| 35:BA:221:A:H61   | 35:BA:265:A:H8     | 1.50                     | 0.57              |
| 35:BA:462:C:C2'   | 35:BA:463:G:C5'    | 2.75                     | 0.57              |
| 35:BA:862:G:H2'   | 35:BA:863:A:O4'    | 2.04                     | 0.57              |
| 35:BA:90:U:O2'    | 35:BA:92:A:OP2     | 2.21                     | 0.57              |
| 35:BA:963:U:HO2'  | 35:BA:964:C:H5'    | 1.64                     | 0.57              |
| 36:BB:2:C:H2'     | 36:BB:3:C:C6       | 2.39                     | 0.57              |
| 42:BH:89:ILE:HG13 | 42:BH:89:ILE:O     | 2.04                     | 0.57              |
| 46:BN:56:ASN:C    | 46:BN:57:ALA:O     | 2.42                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2690:C:OP2   | 50:BR:14:SER:HB3   | 2.04                     | 0.57              |
| 51:BS:30:ARG:CD    | 51:BS:97:ARG:HG2   | 2.32                     | 0.57              |
| 54:BV:5:VAL:HG22   | 54:BV:6:LYS:N      | 2.20                     | 0.57              |
| 1:AA:1296:C:H5'    | 1:AA:1302:U:O4     | 2.05                     | 0.57              |
| 1:AA:1385:G:C2     | 1:AA:1386:G:C4     | 2.93                     | 0.57              |
| 1:AA:937:A:C2'     | 1:AA:938:A:H5'     | 2.35                     | 0.57              |
| 2:AB:231:GLU:CB    | 2:AB:232:PRO:HD2   | 2.20                     | 0.57              |
| 2:AB:239:VAL:HG12  | 2:AB:239:VAL:O     | 2.03                     | 0.57              |
| 7:AG:48:LYS:CG     | 7:AG:49:ILE:N      | 2.67                     | 0.57              |
| 7:AG:48:LYS:HG3    | 7:AG:49:ILE:HG23   | 1.84                     | 0.57              |
| 7:AG:76:ARG:O      | 7:AG:77:SER:HB2    | 2.05                     | 0.57              |
| 16:AP:20:VAL:HG22  | 16:AP:21:VAL:N     | 2.18                     | 0.57              |
| 24:AY:357:ARG:NH1  | 24:AY:366:VAL:HG11 | 2.20                     | 0.57              |
| 25:B0:20:ARG:HG2   | 25:B0:20:ARG:HH11  | 1.68                     | 0.57              |
| 33:B8:37:SER:O     | 33:B8:41:ILE:HG22  | 2.05                     | 0.57              |
| 35:BA:1423:G:O2'   | 35:BA:1424:G:C5'   | 2.30                     | 0.57              |
| 35:BA:1889:A:N1    | 35:BA:2234:G:H1'   | 2.19                     | 0.57              |
| 35:BA:1945:G:C4    | 35:BA:1946:U:C5    | 2.92                     | 0.57              |
| 35:BA:2397:G:O2'   | 35:BA:2398:U:H5'   | 2.05                     | 0.57              |
| 33:B8:62:LEU:CD1   | 35:BA:242:G:H5''   | 2.15                     | 0.57              |
| 35:BA:248:G:H2'    | 35:BA:249:C:OP1    | 2.04                     | 0.57              |
| 35:BA:2662:A:H2'   | 35:BA:2663:G:O4'   | 2.04                     | 0.57              |
| 35:BA:651:G:O6     | 35:BA:652:C:N4     | 2.38                     | 0.57              |
| 35:BA:81:G:H21     | 57:BY:2:ARG:NH1    | 2.02                     | 0.57              |
| 39:BE:8:LYS:HE2    | 39:BE:192:ASN:ND2  | 2.20                     | 0.57              |
| 41:BG:152:LEU:CD2  | 41:BG:152:LEU:H    | 2.17                     | 0.57              |
| 35:BA:1131:G:N2    | 46:BN:73:THR:HG21  | 2.19                     | 0.57              |
| 1:AA:1003:G:C2     | 1:AA:1004:A:H1'    | 2.39                     | 0.57              |
| 1:AA:493:G:H8      | 1:AA:493:G:O5'     | 1.87                     | 0.57              |
| 1:AA:518:C:H4'     | 1:AA:519:C:H5''    | 1.87                     | 0.57              |
| 1:AA:649:G:O2'     | 1:AA:650:G:H5'     | 2.05                     | 0.57              |
| 3:AC:14:ILE:O      | 3:AC:15:THR:HB     | 2.03                     | 0.57              |
| 3:AC:195:VAL:O     | 3:AC:196:LEU:HD22  | 2.04                     | 0.57              |
| 10:AJ:38:ILE:HG12  | 10:AJ:71:LEU:HB3   | 1.87                     | 0.57              |
| 24:AY:316:ILE:CD1  | 24:AY:326:THR:HG23 | 2.35                     | 0.57              |
| 35:BA:1771:C:C1'   | 35:BA:1786:A:C8    | 2.87                     | 0.57              |
| 35:BA:1902:C:C1'   | 38:BD:244:ARG:HB2  | 2.35                     | 0.57              |
| 35:BA:2052:G:H4'   | 39:BE:143:ASN:O    | 2.05                     | 0.57              |
| 35:BA:2123:G:C6    | 35:BA:2176:A:C6    | 2.93                     | 0.57              |
| 35:BA:2409:G:H2'   | 35:BA:2410:G:C8    | 2.39                     | 0.57              |
| 35:BA:271(G):C:O2' | 35:BA:271(H):G:H5' | 2.05                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:462:C:H2'    | 35:BA:463:G:C5'   | 2.32                     | 0.57              |
| 35:BA:598:G:H5'    | 48:BP:15:ARG:HB3  | 1.87                     | 0.57              |
| 35:BA:599:G:O2'    | 35:BA:600:G:H5'   | 2.05                     | 0.57              |
| 35:BA:702:G:H2'    | 35:BA:703:U:C5'   | 2.35                     | 0.57              |
| 38:BD:176:ARG:HG2  | 38:BD:176:ARG:NH1 | 2.20                     | 0.57              |
| 40:BF:138:GLU:O    | 40:BF:141:ALA:HB3 | 2.05                     | 0.57              |
| 40:BF:134:GLY:HA2  | 40:BF:166:ALA:HB2 | 1.86                     | 0.57              |
| 41:BG:77:ILE:HG21  | 41:BG:82:LEU:H    | 1.70                     | 0.57              |
| 42:BH:156:ALA:O    | 42:BH:158:HIS:CD2 | 2.54                     | 0.57              |
| 35:BA:832:G:OP1    | 48:BP:40:SER:HB3  | 2.04                     | 0.57              |
| 49:BQ:74:TYR:HD1   | 49:BQ:75:THR:N    | 2.03                     | 0.57              |
| 51:BS:88:ASP:CG    | 51:BS:89:ARG:H    | 2.07                     | 0.57              |
| 52:BT:30:VAL:HB    | 52:BT:31:SER:CB   | 2.27                     | 0.57              |
| 53:BU:83:LEU:HD12  | 53:BU:88:ILE:HD11 | 1.86                     | 0.57              |
| 54:BV:79:VAL:HG12  | 54:BV:79:VAL:O    | 2.04                     | 0.57              |
| 58:BZ:44:PHE:C     | 58:BZ:44:PHE:CD1  | 2.79                     | 0.57              |
| 1:AA:1447:A:C2'    | 1:AA:1452:C:O5'   | 2.53                     | 0.57              |
| 1:AA:60:A:H1'      | 1:AA:61:G:C1'     | 2.34                     | 0.57              |
| 1:AA:986:A:H2'     | 1:AA:987:G:C8     | 2.39                     | 0.57              |
| 1:AA:992:U:O2      | 1:AA:992:U:H2'    | 2.05                     | 0.57              |
| 10:AJ:8:LEU:HD13   | 10:AJ:70:ARG:HB2  | 1.87                     | 0.57              |
| 16:AP:28:ARG:NH1   | 16:AP:29:ASP:OD1  | 2.38                     | 0.57              |
| 18:AR:58:LEU:HD22  | 18:AR:62:GLU:HB3  | 1.86                     | 0.57              |
| 19:AS:26:GLY:O     | 19:AS:27:GLU:HG3  | 2.04                     | 0.57              |
| 24:AY:81:ILE:HG22  | 24:AY:82:ILE:H    | 1.69                     | 0.57              |
| 24:AY:9:LEU:C      | 24:AY:9:LEU:HD23  | 2.26                     | 0.57              |
| 25:B0:69:PHE:CD2   | 25:B0:79:VAL:CG2  | 2.88                     | 0.57              |
| 29:B4:13:ARG:N     | 29:B4:24:THR:HG23 | 2.19                     | 0.57              |
| 31:B6:8:LYS:HE3    | 31:B6:25:LYS:HG3  | 1.87                     | 0.57              |
| 35:BA:1062:G:H2'   | 35:BA:1063:G:H8   | 1.70                     | 0.57              |
| 35:BA:1088:A:N3    | 35:BA:1088:A:H3'  | 2.20                     | 0.57              |
| 35:BA:1119:C:C2'   | 35:BA:1120:G:C5'  | 2.74                     | 0.57              |
| 35:BA:1316:U:H2'   | 35:BA:1317:A:C8   | 2.40                     | 0.57              |
| 35:BA:1422:G:C6    | 35:BA:1423:G:C5   | 2.92                     | 0.57              |
| 35:BA:1721:G:N3    | 35:BA:1721:G:H5'  | 2.19                     | 0.57              |
| 30:B5:2:ALA:CA     | 35:BA:2015:A:H1'  | 2.31                     | 0.57              |
| 35:BA:2118:U:O4    | 35:BA:2149:G:H1'  | 2.04                     | 0.57              |
| 35:BA:271(L):U:H4' | 35:BA:271(M):G:N7 | 2.19                     | 0.57              |
| 35:BA:2790:A:N3    | 35:BA:2790:A:H2'  | 2.20                     | 0.57              |
| 35:BA:852:G:O2'    | 35:BA:853:G:H5'   | 2.04                     | 0.57              |
| 37:BC:124:VAL:HG13 | 37:BC:125:GLY:N   | 2.20                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BD:142:VAL:HG23 | 38:BD:192:THR:O    | 2.04                     | 0.57              |
| 39:BE:2:LYS:HD3    | 39:BE:95:ILE:HG22  | 1.86                     | 0.57              |
| 35:BA:470:A:OP1    | 40:BF:59:TYR:HE1   | 1.88                     | 0.57              |
| 42:BH:5:GLY:CA     | 42:BH:69:ARG:HD3   | 2.35                     | 0.57              |
| 1:AA:314:C:HO2'    | 1:AA:315:A:H5'     | 1.70                     | 0.56              |
| 3:AC:117:ALA:HB2   | 3:AC:200:ALA:HB3   | 1.87                     | 0.56              |
| 3:AC:12:LEU:O      | 3:AC:14:ILE:N      | 2.38                     | 0.56              |
| 4:AD:3:ARG:HE      | 4:AD:5:ILE:CG1     | 2.18                     | 0.56              |
| 19:AS:42:PRO:C     | 19:AS:44:MET:H     | 2.09                     | 0.56              |
| 19:AS:63:THR:CG2   | 19:AS:64:GLU:H     | 2.07                     | 0.56              |
| 24:AY:183:MET:O    | 24:AY:201:ILE:HD11 | 2.05                     | 0.56              |
| 24:AY:297:GLU:O    | 24:AY:297:GLU:HG3  | 2.05                     | 0.56              |
| 24:AY:99:ARG:HH11  | 24:AY:401:SER:C    | 2.08                     | 0.56              |
| 28:B3:50:VAL:O     | 28:B3:54:VAL:HG13  | 2.05                     | 0.56              |
| 30:B5:51:TYR:O     | 30:B5:52:TYR:C     | 2.37                     | 0.56              |
| 31:B6:15:GLU:HB2   | 31:B6:20:ASN:HB3   | 1.85                     | 0.56              |
| 35:BA:1427:A:H1'   | 35:BA:1428:C:OP2   | 2.05                     | 0.56              |
| 35:BA:1540:U:O3'   | 35:BA:1541:G:H3'   | 2.05                     | 0.56              |
| 35:BA:174:C:H5'    | 35:BA:175:G:OP2    | 2.05                     | 0.56              |
| 35:BA:1800:C:OP1   | 38:BD:266:SER:OG   | 2.18                     | 0.56              |
| 35:BA:2668:G:O2'   | 35:BA:2669:G:H5'   | 2.05                     | 0.56              |
| 35:BA:604:G:O2'    | 35:BA:605:C:C5'    | 2.48                     | 0.56              |
| 40:BF:192:LEU:CD2  | 40:BF:194:MET:HG3  | 2.35                     | 0.56              |
| 41:BG:114:ILE:O    | 41:BG:114:ILE:HG23 | 2.04                     | 0.56              |
| 41:BG:84:LYS:HG3   | 41:BG:84:LYS:O     | 2.04                     | 0.56              |
| 43:BJ:67:UNK:C     | 43:BJ:69:UNK:H     | 2.17                     | 0.56              |
| 47:BO:13:ASN:N     | 47:BO:13:ASN:HD22  | 2.01                     | 0.56              |
| 1:AA:189:G:O2'     | 1:AA:189(A):C:H5'  | 2.05                     | 0.56              |
| 1:AA:511:C:O2'     | 1:AA:512:U:H5''    | 2.05                     | 0.56              |
| 1:AA:684:A:O2'     | 11:AK:39:PRO:O     | 2.21                     | 0.56              |
| 1:AA:1100:C:C4     | 2:AB:96:ARG:NH2    | 2.74                     | 0.56              |
| 9:AI:24:GLY:O      | 9:AI:26:VAL:N      | 2.38                     | 0.56              |
| 10:AJ:54:PHE:C     | 10:AJ:55:LYS:HG3   | 2.25                     | 0.56              |
| 13:AM:39:ILE:HD11  | 13:AM:56:LEU:HB2   | 1.87                     | 0.56              |
| 1:AA:190:U:C2      | 20:AT:105:SER:HB2  | 2.40                     | 0.56              |
| 26:B1:45:ASN:ND2   | 26:B1:47:GLN:HE21  | 2.02                     | 0.56              |
| 31:B6:52:VAL:HG22  | 31:B6:53:LYS:N     | 2.14                     | 0.56              |
| 35:BA:1213:A:O2'   | 35:BA:1214:A:H5'   | 2.04                     | 0.56              |
| 35:BA:1441:G:O2'   | 35:BA:1442:G:H5'   | 2.04                     | 0.56              |
| 35:BA:1465:G:H5'   | 35:BA:1528:A:H1'   | 1.87                     | 0.56              |
| 35:BA:16:G:H2'     | 35:BA:17:G:H5'     | 1.87                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:1771:C:O4'  | 35:BA:1786:A:C8    | 2.58                     | 0.56              |
| 35:BA:1789:A:OP2  | 38:BD:222:ARG:NH1  | 2.36                     | 0.56              |
| 35:BA:197:A:H8    | 35:BA:197:A:H5'    | 1.68                     | 0.56              |
| 35:BA:2306:C:N4   | 35:BA:2311:A:N7    | 2.53                     | 0.56              |
| 35:BA:2610:C:H4'  | 35:BA:2611:U:OP2   | 2.05                     | 0.56              |
| 35:BA:272(I):U:C6 | 35:BA:272(I):U:H5' | 2.30                     | 0.56              |
| 35:BA:93:G:H2'    | 35:BA:94:C:C6      | 2.40                     | 0.56              |
| 37:BC:102:GLN:C   | 37:BC:104:ILE:N    | 2.58                     | 0.56              |
| 37:BC:133:GLY:N   | 37:BC:134:PRO:HD2  | 2.19                     | 0.56              |
| 41:BG:7:LEU:HB2   | 41:BG:104:GLU:OE1  | 2.05                     | 0.56              |
| 41:BG:66:GLN:NE2  | 41:BG:92:VAL:CG2   | 2.67                     | 0.56              |
| 48:BP:115:LEU:CG  | 48:BP:116:GLY:N    | 2.68                     | 0.56              |
| 35:BA:833:U:H4'   | 48:BP:52:GLU:H     | 1.65                     | 0.56              |
| 51:BS:102:ALA:HB3 | 51:BS:103:GLU:OE1  | 2.05                     | 0.56              |
| 51:BS:58:LEU:HD21 | 51:BS:68:GLN:HB2   | 1.87                     | 0.56              |
| 35:BA:896:A:H5'   | 58:BZ:146:ILE:HD12 | 1.88                     | 0.56              |
| 1:AA:1001:A:H2'   | 1:AA:1001:A:N3     | 2.20                     | 0.56              |
| 1:AA:1525:G:O2'   | 1:AA:1526:G:H5'    | 2.04                     | 0.56              |
| 1:AA:197:A:N6     | 1:AA:221:C:C4'     | 2.67                     | 0.56              |
| 1:AA:882:C:O2'    | 1:AA:883:C:H5'     | 2.06                     | 0.56              |
| 3:AC:131:ARG:O    | 3:AC:134:ILE:HB    | 2.05                     | 0.56              |
| 4:AD:145:GLU:OE1  | 4:AD:182:LYS:HD3   | 2.05                     | 0.56              |
| 35:BA:1077:A:C6   | 35:BA:1078:U:H1'   | 2.40                     | 0.56              |
| 35:BA:1416:G:HO2' | 35:BA:1417:C:H5    | 0.70                     | 0.56              |
| 35:BA:1461:G:C6   | 35:BA:1462:C:C4    | 2.93                     | 0.56              |
| 35:BA:2408:U:C2   | 35:BA:2409:G:N7    | 2.73                     | 0.56              |
| 35:BA:412:A:N7    | 35:BA:2411:A:H2    | 2.03                     | 0.56              |
| 35:BA:492:A:H2'   | 35:BA:493:G:O4'    | 2.04                     | 0.56              |
| 37:BC:88:GLU:HB2  | 37:BC:92:ALA:HB3   | 1.85                     | 0.56              |
| 40:BF:160:ASN:ND2 | 40:BF:162:LEU:HD13 | 2.14                     | 0.56              |
| 40:BF:175:THR:C   | 40:BF:176:LEU:HD12 | 2.24                     | 0.56              |
| 42:BH:166:GLY:O   | 42:BH:167:GLU:CB   | 2.53                     | 0.56              |
| 44:BK:56:UNK:O    | 44:BK:67:UNK:HA    | 2.05                     | 0.56              |
| 47:BO:35:VAL:HG23 | 47:BO:69:ILE:HD11  | 1.86                     | 0.56              |
| 55:BW:24:ILE:O    | 55:BW:71:VAL:HG21  | 2.04                     | 0.56              |
| 57:BY:17:SER:CA   | 57:BY:71:LYS:HE2   | 2.35                     | 0.56              |
| 57:BY:39:VAL:HG12 | 57:BY:40:GLU:N     | 2.21                     | 0.56              |
| 1:AA:123:C:OP1    | 1:AA:312:C:H5''    | 2.05                     | 0.56              |
| 1:AA:490:G:C4     | 1:AA:491:G:C8      | 2.93                     | 0.56              |
| 1:AA:862:C:O2'    | 1:AA:863:U:H5''    | 2.06                     | 0.56              |
| 12:AL:27:LEU:HD13 | 12:AL:28:LYS:HG3   | 1.86                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:AV:73:A:C2'     | 22:AV:74:C:H5'    | 2.36                     | 0.56              |
| 24:AY:534:ILE:CD1  | 24:AY:570:GLY:HA3 | 2.30                     | 0.56              |
| 26:B1:45:ASN:HD21  | 35:BA:2090:G:N2   | 1.93                     | 0.56              |
| 29:B4:32:TYR:CE2   | 29:B4:34:GLU:HB2  | 2.40                     | 0.56              |
| 33:B8:30:ARG:NE    | 33:B8:30:ARG:HA   | 2.19                     | 0.56              |
| 33:B8:48:PHE:C     | 33:B8:49:VAL:HG22 | 2.25                     | 0.56              |
| 35:BA:1047:G:H2'   | 35:BA:1110:G:H21  | 1.69                     | 0.56              |
| 35:BA:1137:G:C2'   | 35:BA:1138:G:H5'  | 2.33                     | 0.56              |
| 35:BA:1268:A:H2'   | 35:BA:1269:A:O4'  | 2.06                     | 0.56              |
| 35:BA:1688:U:H1'   | 35:BA:1701:A:C6   | 2.40                     | 0.56              |
| 35:BA:2401:U:H3'   | 35:BA:2402:C:C6   | 2.40                     | 0.56              |
| 35:BA:258:G:C2'    | 35:BA:259:G:H5'   | 2.35                     | 0.56              |
| 35:BA:652:C:N1     | 35:BA:653:A:C8    | 2.73                     | 0.56              |
| 35:BA:693:C:O2'    | 35:BA:694:U:C5'   | 2.50                     | 0.56              |
| 35:BA:697:C:H2'    | 35:BA:698:C:H5'   | 1.84                     | 0.56              |
| 37:BC:109:MET:HA   | 37:BC:111:PHE:CZ  | 2.40                     | 0.56              |
| 38:BD:211:ARG:HD3  | 38:BD:214:TRP:CZ3 | 2.41                     | 0.56              |
| 35:BA:1257:C:H4'   | 40:BF:83:PHE:CD2  | 2.40                     | 0.56              |
| 41:BG:110:ALA:CB   | 41:BG:142:PRO:HB3 | 2.35                     | 0.56              |
| 49:BQ:14:ARG:HG2   | 49:BQ:14:ARG:HH11 | 1.70                     | 0.56              |
| 58:BZ:103:ARG:HH11 | 58:BZ:103:ARG:HB2 | 1.70                     | 0.56              |
| 1:AA:1175:G:H2'    | 1:AA:1176:A:H5'   | 1.87                     | 0.56              |
| 1:AA:1366:C:O2'    | 1:AA:1367:C:H5'   | 2.05                     | 0.56              |
| 1:AA:685:G:H8      | 1:AA:685:G:O5'    | 1.87                     | 0.56              |
| 1:AA:89:C:C2       | 1:AA:90:U:H5      | 2.23                     | 0.56              |
| 2:AB:19:HIS:NE2    | 2:AB:206:ASP:HB2  | 2.20                     | 0.56              |
| 4:AD:126:ILE:HD12  | 4:AD:126:ILE:N    | 2.20                     | 0.56              |
| 13:AM:97:PRO:HB2   | 13:AM:101:GLN:NE2 | 2.19                     | 0.56              |
| 24:AY:151:ARG:O    | 24:AY:155:GLU:HB2 | 2.05                     | 0.56              |
| 24:AY:631:ILE:HA   | 24:AY:645:ALA:CB  | 2.34                     | 0.56              |
| 24:AY:5:VAL:HG13   | 24:AY:6:GLU:N     | 2.21                     | 0.56              |
| 29:B4:12:ALA:N     | 29:B4:24:THR:CB   | 2.55                     | 0.56              |
| 29:B4:48:ARG:HG2   | 29:B4:48:ARG:HH11 | 1.70                     | 0.56              |
| 33:B8:28:GLY:O     | 33:B8:30:ARG:N    | 2.35                     | 0.56              |
| 35:BA:1445:A:C8    | 35:BA:1460:A:C6   | 2.94                     | 0.56              |
| 35:BA:2106:G:H8    | 35:BA:2106:G:H5'  | 1.70                     | 0.56              |
| 35:BA:2410:G:N2    | 35:BA:2411:A:H1'  | 2.20                     | 0.56              |
| 35:BA:252:G:O2'    | 35:BA:253:C:H5'   | 2.05                     | 0.56              |
| 35:BA:965:C:H2'    | 35:BA:966:G:H5'   | 1.87                     | 0.56              |
| 41:BG:128:ARG:O    | 41:BG:128:ARG:HG3 | 2.05                     | 0.56              |
| 41:BG:52:ILE:O     | 41:BG:53:LEU:HG   | 2.06                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:BX:11:PRO:HB3   | 56:BX:92:LEU:HD21  | 1.86                     | 0.56              |
| 58:BZ:56:VAL:HG13  | 58:BZ:69:THR:O     | 2.05                     | 0.56              |
| 1:AA:1077:G:C6     | 1:AA:1081:G:O6     | 2.59                     | 0.56              |
| 1:AA:1488:G:C2'    | 1:AA:1489:G:H5'    | 2.35                     | 0.56              |
| 1:AA:197:A:N6      | 1:AA:221:C:C5'     | 2.68                     | 0.56              |
| 1:AA:501:C:OP1     | 12:AL:117:ARG:NH2  | 2.37                     | 0.56              |
| 1:AA:552:U:H4'     | 12:AL:86:ARG:HG2   | 1.88                     | 0.56              |
| 2:AB:204:ASN:ND2   | 2:AB:205:ASP:N     | 2.50                     | 0.56              |
| 2:AB:20:GLU:CA     | 2:AB:20:GLU:OE1    | 2.54                     | 0.56              |
| 3:AC:190:ARG:HH11  | 3:AC:190:ARG:HG3   | 1.71                     | 0.56              |
| 13:AM:65:LYS:HD2   | 13:AM:73:GLU:HG3   | 1.86                     | 0.56              |
| 17:AQ:40:LYS:HD3   | 17:AQ:42:TYR:OH    | 2.05                     | 0.56              |
| 24:AY:38:ARG:HH22  | 24:AY:270:GLN:NE2  | 2.03                     | 0.56              |
| 24:AY:431:LEU:HD11 | 24:AY:465:ARG:HH12 | 1.71                     | 0.56              |
| 35:BA:1493:C:H2'   | 35:BA:1493:C:O2    | 2.05                     | 0.56              |
| 35:BA:1486:A:N1    | 35:BA:1504:C:N4    | 2.53                     | 0.56              |
| 35:BA:1893:C:O2'   | 35:BA:1894:C:H5'   | 2.06                     | 0.56              |
| 35:BA:2363:C:C2    | 35:BA:2364:C:C5    | 2.93                     | 0.56              |
| 35:BA:2756:U:C1'   | 35:BA:2757:A:OP2   | 2.47                     | 0.56              |
| 35:BA:692:C:H2'    | 35:BA:693:C:C5'    | 2.36                     | 0.56              |
| 35:BA:885:C:O2     | 35:BA:885:C:H2'    | 2.05                     | 0.56              |
| 35:BA:89:G:H3'     | 35:BA:90:U:H5'     | 1.88                     | 0.56              |
| 37:BC:74:ARG:HG2   | 37:BC:111:PHE:HA   | 1.87                     | 0.56              |
| 35:BA:1797:C:O2'   | 38:BD:259:THR:HG22 | 2.04                     | 0.56              |
| 38:BD:43:ARG:HH11  | 38:BD:44:ASN:CG    | 2.08                     | 0.56              |
| 39:BE:101:ARG:HD2  | 39:BE:169:ASN:ND2  | 2.19                     | 0.56              |
| 40:BF:132:VAL:HG22 | 40:BF:133:ASN:N    | 2.20                     | 0.56              |
| 1:AA:322:C:H41     | 1:AA:328:C:H6      | 1.53                     | 0.56              |
| 1:AA:327:A:C2      | 1:AA:329:A:C4      | 2.94                     | 0.56              |
| 1:AA:36:C:O5'      | 1:AA:36:C:H6       | 1.88                     | 0.56              |
| 1:AA:555:C:N3      | 1:AA:556:C:C4      | 2.74                     | 0.56              |
| 1:AA:961:U:H2'     | 1:AA:961:U:OP1     | 2.05                     | 0.56              |
| 2:AB:145:LEU:O     | 2:AB:149:LEU:CB    | 2.32                     | 0.56              |
| 29:B4:42:PHE:N     | 29:B4:42:PHE:HD1   | 2.03                     | 0.56              |
| 35:BA:108:U:C2'    | 35:BA:109:G:C5'    | 2.83                     | 0.56              |
| 35:BA:1137:G:O2'   | 35:BA:1138:G:C5'   | 2.38                     | 0.56              |
| 35:BA:145:G:O2'    | 35:BA:146:G:H5'    | 2.05                     | 0.56              |
| 35:BA:1821:A:H2'   | 35:BA:1822:G:H8    | 1.71                     | 0.56              |
| 35:BA:2001:A:H2'   | 35:BA:2002:G:C8    | 2.40                     | 0.56              |
| 35:BA:2361:A:H2'   | 35:BA:2362:G:H5'   | 1.86                     | 0.56              |
| 35:BA:2439:A:C8    | 35:BA:2439:A:H5'   | 2.41                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:2556:C:C2'  | 35:BA:2557:G:O5'   | 2.52                     | 0.56              |
| 35:BA:256:A:O2'   | 35:BA:257:A:H5'    | 2.04                     | 0.56              |
| 35:BA:259:G:O2'   | 35:BA:260:G:C5'    | 2.36                     | 0.56              |
| 35:BA:2699:C:O2'  | 35:BA:2700:C:H5'   | 2.06                     | 0.56              |
| 35:BA:692:C:O2'   | 35:BA:693:C:C5'    | 2.45                     | 0.56              |
| 39:BE:201:THR:C   | 39:BE:202:LYS:HD2  | 2.26                     | 0.56              |
| 39:BE:34:VAL:HG21 | 39:BE:78:LEU:CD2   | 2.35                     | 0.56              |
| 40:BF:80:ALA:O    | 40:BF:81:PRO:C     | 2.43                     | 0.56              |
| 41:BG:127:GLY:C   | 41:BG:129:GLY:H    | 2.08                     | 0.56              |
| 41:BG:68:PRO:HB3  | 41:BG:92:VAL:HB    | 1.87                     | 0.56              |
| 35:BA:2751:G:C6   | 42:BH:1:MET:HG2    | 2.41                     | 0.56              |
| 52:BT:41:ARG:HD3  | 52:BT:41:ARG:C     | 2.26                     | 0.56              |
| 53:BU:52:ARG:NH1  | 53:BU:52:ARG:HB3   | 2.20                     | 0.56              |
| 57:BY:8:LYS:N     | 57:BY:8:LYS:CD     | 2.65                     | 0.56              |
| 1:AA:39:G:N7      | 1:AA:547:A:H8      | 2.03                     | 0.56              |
| 1:AA:614:A:H2'    | 1:AA:615:C:C6      | 2.41                     | 0.56              |
| 4:AD:36:ARG:HA    | 4:AD:38:TYR:CE1    | 2.40                     | 0.56              |
| 10:AJ:35:SER:OG   | 10:AJ:73:ASP:HB2   | 2.05                     | 0.56              |
| 26:B1:72:GLU:O    | 26:B1:76:ARG:HG3   | 2.05                     | 0.56              |
| 35:BA:1804:C:O2'  | 35:BA:1805:U:H5'   | 2.05                     | 0.56              |
| 35:BA:1806:C:C2'  | 35:BA:1807:G:C5'   | 2.84                     | 0.56              |
| 35:BA:747:U:N1    | 35:BA:2613:U:O4    | 2.35                     | 0.56              |
| 35:BA:2784:C:H1'  | 39:BE:37:ARG:NH1   | 2.21                     | 0.56              |
| 35:BA:30:G:OP2    | 53:BU:5:LYS:NZ     | 2.39                     | 0.56              |
| 35:BA:659:C:H4'   | 40:BF:100:THR:O    | 2.06                     | 0.56              |
| 39:BE:14:ILE:HD11 | 39:BE:173:VAL:HG11 | 1.86                     | 0.56              |
| 41:BG:52:ILE:HB   | 41:BG:54:GLU:HG3   | 1.88                     | 0.56              |
| 41:BG:6:ALA:CB    | 41:BG:105:LYS:NZ   | 2.69                     | 0.56              |
| 46:BN:45:ASN:N    | 46:BN:45:ASN:HD22  | 2.03                     | 0.56              |
| 48:BP:96:THR:O    | 48:BP:100:LEU:HD23 | 2.05                     | 0.56              |
| 51:BS:53:SER:OG   | 51:BS:54:LEU:N     | 2.38                     | 0.56              |
| 51:BS:89:ARG:HB3  | 51:BS:92:TYR:HB3   | 1.87                     | 0.56              |
| 57:BY:52:SER:O    | 57:BY:53:PRO:C     | 2.44                     | 0.56              |
| 1:AA:118:U:H3'    | 1:AA:288:A:H61     | 1.69                     | 0.56              |
| 1:AA:1275:A:O2'   | 1:AA:1276:G:H5'    | 2.05                     | 0.56              |
| 1:AA:154:C:H2'    | 1:AA:155:C:C6      | 2.41                     | 0.56              |
| 1:AA:490:G:HO2'   | 1:AA:491:G:H5'     | 1.68                     | 0.56              |
| 1:AA:592:G:H2'    | 1:AA:593:G:H5'     | 1.86                     | 0.56              |
| 1:AA:61:G:H2'     | 1:AA:62:U:C6       | 2.41                     | 0.56              |
| 1:AA:698:G:O2'    | 1:AA:699:C:H5'     | 2.05                     | 0.56              |
| 4:AD:31:CYS:C     | 4:AD:33:MET:H      | 2.08                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AH:10:LEU:HD22   | 8:AH:83:ILE:HD11   | 1.88                     | 0.56              |
| 16:AP:45:THR:HG23  | 16:AP:46:PRO:HD2   | 1.87                     | 0.56              |
| 24:AY:686:LYS:HD3  | 24:AY:686:LYS:O    | 2.06                     | 0.56              |
| 35:BA:54:G:C6      | 35:BA:117:G:N2     | 2.74                     | 0.56              |
| 35:BA:1222:C:H2'   | 35:BA:1223:G:C5'   | 2.33                     | 0.56              |
| 35:BA:1459:G:N3    | 35:BA:1459:G:C3'   | 2.68                     | 0.56              |
| 35:BA:644:A:H2     | 35:BA:2369:A:H1'   | 1.69                     | 0.56              |
| 35:BA:627:A:H62    | 48:BP:116:GLY:HA2  | 1.70                     | 0.56              |
| 35:BA:925:C:C3'    | 35:BA:926:A:H5''   | 2.36                     | 0.56              |
| 38:BD:106:ILE:HG12 | 38:BD:106:ILE:O    | 2.05                     | 0.56              |
| 41:BG:83:ARG:C     | 41:BG:85:GLY:H     | 2.08                     | 0.56              |
| 42:BH:137:ASP:O    | 42:BH:138:LYS:HB2  | 2.05                     | 0.56              |
| 46:BN:2:LYS:HE3    | 46:BN:2:LYS:N      | 2.19                     | 0.56              |
| 51:BS:97:ARG:C     | 51:BS:97:ARG:NE    | 2.58                     | 0.56              |
| 52:BT:6:LEU:O      | 52:BT:10:VAL:HG23  | 2.06                     | 0.56              |
| 57:BY:42:VAL:HG12  | 57:BY:42:VAL:O     | 2.06                     | 0.56              |
| 57:BY:43:ASN:HA    | 57:BY:64:GLU:HA    | 1.88                     | 0.56              |
| 1:AA:1036:G:H5''   | 1:AA:1037:C:C5     | 2.41                     | 0.56              |
| 1:AA:1179:A:H2'    | 1:AA:1180:A:C5'    | 2.35                     | 0.56              |
| 1:AA:1239:A:H4'    | 1:AA:1240:U:O5'    | 2.06                     | 0.56              |
| 1:AA:1314:C:H2'    | 1:AA:1315:U:C6     | 2.41                     | 0.56              |
| 1:AA:1386:G:C2     | 1:AA:1387:G:C8     | 2.94                     | 0.56              |
| 1:AA:1490:C:C3'    | 1:AA:1491:G:H5'    | 2.34                     | 0.56              |
| 1:AA:788:U:N3      | 1:AA:792:A:O2'     | 2.34                     | 0.56              |
| 1:AA:953:G:H2'     | 1:AA:954:G:O4'     | 2.06                     | 0.56              |
| 1:AA:967:C:H4'     | 9:AI:125:TYR:CE1   | 2.36                     | 0.56              |
| 2:AB:59:GLU:HB2    | 2:AB:221:LEU:HD21  | 1.86                     | 0.56              |
| 7:AG:152:ALA:HB1   | 7:AG:155:ARG:HH21  | 1.70                     | 0.56              |
| 13:AM:40:ASN:HD22  | 13:AM:43:THR:CG2   | 2.18                     | 0.56              |
| 15:AO:17:ARG:NH1   | 15:AO:17:ARG:HG3   | 2.20                     | 0.56              |
| 24:AY:348:ARG:HG3  | 24:AY:348:ARG:HH11 | 1.69                     | 0.56              |
| 24:AY:506:GLN:HB2  | 24:AY:576:ASP:O    | 2.05                     | 0.56              |
| 30:B5:47:PRO:O     | 30:B5:48:GLU:C     | 2.44                     | 0.56              |
| 35:BA:49:A:O4'     | 35:BA:51:G:C4      | 2.59                     | 0.56              |
| 38:BD:8:PRO:HB3    | 38:BD:14:ARG:CB    | 2.36                     | 0.56              |
| 46:BN:94:HIS:N     | 46:BN:95:PRO:CD    | 2.69                     | 0.56              |
| 48:BP:115:LEU:HA   | 48:BP:134:ALA:HB2  | 1.86                     | 0.56              |
| 48:BP:126:VAL:HG12 | 48:BP:148:LEU:HD11 | 1.88                     | 0.56              |
| 51:BS:54:LEU:C     | 51:BS:56:LEU:H     | 2.07                     | 0.56              |
| 54:BV:55:ALA:CB    | 54:BV:101:GLY:HA2  | 2.35                     | 0.56              |
| 58:BZ:60:GLU:O     | 58:BZ:61:LEU:CB    | 2.54                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1029:C:H42   | 1:AA:1033:G:H1     | 1.54                     | 0.56              |
| 1:AA:1041:A:H2'   | 1:AA:1042:G:H8     | 1.70                     | 0.56              |
| 1:AA:1447:A:H2'   | 1:AA:1452:C:O5'    | 2.06                     | 0.56              |
| 1:AA:1505:G:H4'   | 1:AA:1506:U:H5''   | 1.88                     | 0.56              |
| 1:AA:453:A:O2'    | 1:AA:454:C:C6      | 2.58                     | 0.56              |
| 2:AB:102:LEU:HB3  | 2:AB:180:LEU:HD12  | 1.87                     | 0.56              |
| 2:AB:77:ALA:O     | 2:AB:81:VAL:HG23   | 2.06                     | 0.56              |
| 7:AG:73:MET:HE2   | 7:AG:89:MET:C      | 2.26                     | 0.56              |
| 13:AM:11:ARG:H    | 13:AM:45:VAL:HG21  | 1.70                     | 0.56              |
| 17:AQ:9:VAL:HG11  | 17:AQ:84:LEU:CD1   | 2.36                     | 0.56              |
| 22:AV:39:U:H2'    | 22:AV:40:C:H6      | 1.69                     | 0.56              |
| 22:AV:41:C:H2'    | 22:AV:42:C:H5'     | 1.85                     | 0.56              |
| 24:AY:228:MET:O   | 24:AY:232:LEU:HD22 | 2.06                     | 0.56              |
| 24:AY:7:TYR:CE2   | 24:AY:370:LYS:HD2  | 2.40                     | 0.56              |
| 35:BA:1695:G:H5'' | 35:BA:1695:G:N3    | 2.20                     | 0.56              |
| 39:BE:16:ARG:NH2  | 39:BE:171:GLU:OE2  | 2.39                     | 0.56              |
| 41:BG:34:LEU:HG   | 41:BG:161:THR:HG22 | 1.87                     | 0.56              |
| 41:BG:93:THR:O    | 41:BG:94:LEU:HB2   | 2.06                     | 0.56              |
| 48:BP:115:LEU:HB2 | 48:BP:131:SER:OG   | 2.05                     | 0.56              |
| 48:BP:77:ARG:HH11 | 48:BP:77:ARG:HG2   | 1.71                     | 0.56              |
| 52:BT:28:VAL:O    | 52:BT:29:ARG:CB    | 2.51                     | 0.56              |
| 52:BT:38:ASN:ND2  | 52:BT:38:ASN:H     | 2.04                     | 0.56              |
| 53:BU:87:GLY:C    | 53:BU:89:GLU:H     | 2.09                     | 0.56              |
| 54:BV:5:VAL:CG2   | 54:BV:6:LYS:N      | 2.69                     | 0.56              |
| 1:AA:1033:G:H2'   | 1:AA:1034:G:H8     | 1.71                     | 0.55              |
| 1:AA:106:C:C2'    | 1:AA:107:G:C5'     | 2.83                     | 0.55              |
| 1:AA:359:U:H2'    | 1:AA:360:A:C8      | 2.41                     | 0.55              |
| 1:AA:683:G:C6     | 1:AA:684:A:C6      | 2.94                     | 0.55              |
| 1:AA:775:G:O2'    | 1:AA:776:G:C5'     | 2.30                     | 0.55              |
| 1:AA:788:U:C2'    | 1:AA:789:U:C5'     | 2.83                     | 0.55              |
| 1:AA:792:A:H1'    | 1:AA:794:A:N7      | 2.21                     | 0.55              |
| 1:AA:948:C:H6     | 1:AA:948:C:O5'     | 1.89                     | 0.55              |
| 1:AA:959:A:O3'    | 1:AA:960:U:H4'     | 2.06                     | 0.55              |
| 3:AC:164:ARG:HG2  | 3:AC:164:ARG:HH11  | 1.71                     | 0.55              |
| 7:AG:71:PRO:HD3   | 7:AG:103:TRP:CZ3   | 2.41                     | 0.55              |
| 7:AG:83:ALA:HB1   | 7:AG:85:TYR:CZ     | 2.40                     | 0.55              |
| 9:AI:126:SER:O    | 9:AI:127:LYS:CB    | 2.53                     | 0.55              |
| 12:AL:83:VAL:CG1  | 12:AL:100:ILE:HG23 | 2.35                     | 0.55              |
| 19:AS:32:LYS:CB   | 19:AS:50:ALA:HB3   | 2.36                     | 0.55              |
| 20:AT:73:HIS:O    | 20:AT:74:LYS:CG    | 2.48                     | 0.55              |
| 1:AA:1305:G:H5'   | 21:AU:4:GLY:C      | 2.26                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:610:VAL:HG22 | 24:AY:643:ILE:HB   | 1.89                     | 0.55              |
| 25:B0:45:PHE:CE1   | 25:B0:77:ARG:NE    | 2.71                     | 0.55              |
| 29:B4:42:PHE:N     | 29:B4:42:PHE:CD1   | 2.74                     | 0.55              |
| 30:B5:40:LYS:HD3   | 30:B5:46:CYS:HB2   | 1.87                     | 0.55              |
| 35:BA:1192:G:O2'   | 35:BA:1193:G:H5'   | 2.06                     | 0.55              |
| 35:BA:1424:G:H2'   | 35:BA:1425:G:O5'   | 2.06                     | 0.55              |
| 35:BA:49:A:N6      | 35:BA:177:G:C2     | 2.74                     | 0.55              |
| 35:BA:1902:C:C4'   | 38:BD:244:ARG:HB2  | 2.35                     | 0.55              |
| 35:BA:1835:G:H1'   | 35:BA:1931:U:C2    | 2.41                     | 0.55              |
| 35:BA:1970:A:C4'   | 35:BA:1972:A:C1'   | 2.83                     | 0.55              |
| 35:BA:2464:C:O2'   | 35:BA:2465:C:H6    | 1.88                     | 0.55              |
| 35:BA:2610:C:HO2'  | 35:BA:2611:U:P     | 2.27                     | 0.55              |
| 35:BA:848:G:N3     | 35:BA:933:A:H1'    | 2.21                     | 0.55              |
| 35:BA:894:C:O2'    | 35:BA:895:U:H5'    | 2.06                     | 0.55              |
| 36:BB:111:G:O2'    | 36:BB:112:U:H5'    | 2.06                     | 0.55              |
| 36:BB:7:G:C3'      | 36:BB:8:U:H5"      | 2.36                     | 0.55              |
| 37:BC:42:VAL:O     | 37:BC:216:THR:O    | 2.24                     | 0.55              |
| 40:BF:8:GLN:O      | 40:BF:9:ILE:C      | 2.44                     | 0.55              |
| 43:BJ:69:UNK:O     | 43:BJ:70:UNK:O     | 2.24                     | 0.55              |
| 44:BK:128:UNK:O    | 44:BK:130:UNK:N    | 2.39                     | 0.55              |
| 44:BK:28:UNK:O     | 44:BK:29:UNK:C     | 2.52                     | 0.55              |
| 58:BZ:141:VAL:O    | 58:BZ:144:LEU:HD23 | 2.06                     | 0.55              |
| 1:AA:591:U:C2'     | 1:AA:592:G:O5'     | 2.54                     | 0.55              |
| 1:AA:867:G:C2'     | 1:AA:868:C:H5'     | 2.36                     | 0.55              |
| 2:AB:37:ASN:O      | 2:AB:39:ILE:HG13   | 2.06                     | 0.55              |
| 9:AI:3:GLN:OE1     | 9:AI:20:ARG:NH1    | 2.38                     | 0.55              |
| 10:AJ:49:VAL:O     | 10:AJ:60:ARG:HB3   | 2.05                     | 0.55              |
| 24:AY:550:MET:HE1  | 24:AY:563:ILE:HD11 | 1.88                     | 0.55              |
| 24:AY:506:GLN:HG2  | 24:AY:573:HIS:CE1  | 2.41                     | 0.55              |
| 24:AY:264:LEU:CB   | 61:AY:701:GCP:C6   | 2.84                     | 0.55              |
| 24:AY:84:THR:HG23  | 24:AY:85:PRO:N     | 2.20                     | 0.55              |
| 25:B0:33:ALA:N     | 25:B0:64:ASP:OD1   | 2.34                     | 0.55              |
| 35:BA:1216:G:H2'   | 35:BA:1217:C:H5'   | 1.88                     | 0.55              |
| 35:BA:1204:A:N1    | 35:BA:1241:A:C2    | 2.74                     | 0.55              |
| 35:BA:1773:A:O2'   | 35:BA:1774:C:H5'   | 2.03                     | 0.55              |
| 35:BA:1804:C:C2'   | 35:BA:1805:U:H5'   | 2.36                     | 0.55              |
| 35:BA:2182:G:O2'   | 35:BA:2183:C:H5'   | 2.06                     | 0.55              |
| 35:BA:247:G:H2'    | 35:BA:248:G:O5'    | 2.06                     | 0.55              |
| 35:BA:889:C:H2'    | 35:BA:890:A:O4'    | 2.06                     | 0.55              |
| 35:BA:896:A:N3     | 58:BZ:176:PRO:HB3  | 2.21                     | 0.55              |
| 37:BC:129:GLY:O    | 37:BC:131:ILE:N    | 2.38                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:39:ILE:HD11  | 41:BG:155:MET:HG3  | 1.88                     | 0.55              |
| 49:BQ:110:THR:HG23 | 49:BQ:113:GLN:OE1  | 2.06                     | 0.55              |
| 52:BT:42:ILE:O     | 52:BT:42:ILE:HG13  | 2.05                     | 0.55              |
| 55:BW:10:VAL:O     | 55:BW:11:ARG:CB    | 2.54                     | 0.55              |
| 57:BY:55:TYR:N     | 57:BY:56:PRO:HD3   | 2.22                     | 0.55              |
| 58:BZ:100:VAL:HG11 | 58:BZ:137:ILE:HD11 | 1.89                     | 0.55              |
| 1:AA:1396:A:O4'    | 1:AA:1398:A:H1'    | 2.07                     | 0.55              |
| 1:AA:1427:U:H2'    | 1:AA:1428:A:C8     | 2.41                     | 0.55              |
| 1:AA:1505:G:C5'    | 1:AA:1506:U:OP1    | 2.42                     | 0.55              |
| 1:AA:197:A:N6      | 1:AA:221:C:H5''    | 2.21                     | 0.55              |
| 1:AA:356:A:H1'     | 1:AA:368:U:O2'     | 2.06                     | 0.55              |
| 1:AA:588:G:H2'     | 1:AA:589:C:C6      | 2.41                     | 0.55              |
| 1:AA:951:G:O6      | 1:AA:1230:C:C4     | 2.59                     | 0.55              |
| 2:AB:168:THR:HG23  | 2:AB:192:SER:CB    | 2.36                     | 0.55              |
| 3:AC:28:GLN:O      | 3:AC:29:TYR:C      | 2.44                     | 0.55              |
| 4:AD:150:GLU:CG    | 4:AD:151:LYS:H     | 2.19                     | 0.55              |
| 10:AJ:49:VAL:HG23  | 14:AN:41:ARG:HB2   | 1.88                     | 0.55              |
| 24:AY:348:ARG:CG   | 24:AY:348:ARG:HH11 | 2.19                     | 0.55              |
| 35:BA:1041:G:H1    | 35:BA:1114:G:H22   | 1.54                     | 0.55              |
| 35:BA:1297:C:H2'   | 35:BA:1298:C:H6    | 1.71                     | 0.55              |
| 35:BA:1313:U:H2'   | 35:BA:1610:A:C2    | 2.41                     | 0.55              |
| 35:BA:1798:U:O2    | 35:BA:1821:A:C2    | 2.59                     | 0.55              |
| 35:BA:2461:C:H2'   | 35:BA:2462:U:C6    | 2.42                     | 0.55              |
| 35:BA:658:C:H2'    | 35:BA:659:C:H6     | 1.72                     | 0.55              |
| 40:BF:3:GLU:CB     | 40:BF:24:LEU:HG    | 2.36                     | 0.55              |
| 41:BG:11:TYR:OH    | 41:BG:33:ARG:HB3   | 2.07                     | 0.55              |
| 41:BG:54:GLU:O     | 41:BG:57:ALA:HB3   | 2.06                     | 0.55              |
| 44:BK:61:UNK:O     | 44:BK:62:UNK:CB    | 2.54                     | 0.55              |
| 48:BP:23:PRO:C     | 48:BP:33:ARG:NE    | 2.60                     | 0.55              |
| 51:BS:29:PHE:HD1   | 51:BS:30:ARG:N     | 2.04                     | 0.55              |
| 52:BT:28:VAL:HG11  | 52:BT:46:GLU:CG    | 2.36                     | 0.55              |
| 52:BT:34:VAL:CG1   | 52:BT:39:ARG:HG3   | 2.36                     | 0.55              |
| 52:BT:6:LEU:C      | 52:BT:8:LYS:H      | 2.08                     | 0.55              |
| 54:BV:59:ALA:HB2   | 54:BV:96:ILE:HD13  | 1.88                     | 0.55              |
| 1:AA:1048:G:O6     | 1:AA:1210:C:N4     | 2.39                     | 0.55              |
| 1:AA:1282:C:H6     | 1:AA:1282:C:O5'    | 1.89                     | 0.55              |
| 1:AA:186:C:O2'     | 1:AA:187:C:C5'     | 2.48                     | 0.55              |
| 1:AA:495:A:H1'     | 1:AA:496:A:C2'     | 2.36                     | 0.55              |
| 1:AA:91:C:O2       | 1:AA:91:C:H2'      | 2.07                     | 0.55              |
| 2:AB:187:LEU:CG    | 2:AB:187:LEU:O     | 2.52                     | 0.55              |
| 3:AC:120:VAL:C     | 3:AC:122:GLU:H     | 2.09                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:AC:169:ALA:O     | 3:AC:170:GLN:HB2  | 2.05                     | 0.55              |
| 7:AG:121:ALA:O     | 7:AG:125:MET:N    | 2.38                     | 0.55              |
| 12:AL:83:VAL:HG11  | 12:AL:100:ILE:CG1 | 2.35                     | 0.55              |
| 13:AM:56:LEU:HD13  | 13:AM:56:LEU:C    | 2.27                     | 0.55              |
| 14:AN:32:SER:HB3   | 14:AN:41:ARG:CG   | 2.37                     | 0.55              |
| 35:BA:1048:A:H62   | 42:BH:1:MET:HE1   | 1.71                     | 0.55              |
| 35:BA:1142(A):A:C4 | 35:BA:1144:G:N7   | 2.74                     | 0.55              |
| 35:BA:2129:C:N3    | 35:BA:2159:G:N1   | 2.39                     | 0.55              |
| 35:BA:2169:A:H5'   | 37:BC:130:ARG:NH2 | 2.21                     | 0.55              |
| 35:BA:2360:A:O2'   | 35:BA:2361:A:P    | 2.63                     | 0.55              |
| 35:BA:2559:C:C2'   | 35:BA:2560:C:H5'  | 2.36                     | 0.55              |
| 35:BA:657:U:H2'    | 35:BA:658:C:C6    | 2.41                     | 0.55              |
| 38:BD:30:GLU:CG    | 38:BD:63:ARG:NE   | 2.67                     | 0.55              |
| 39:BE:203:LYS:C    | 39:BE:203:LYS:HD2 | 2.26                     | 0.55              |
| 40:BF:110:LEU:HD22 | 40:BF:202:PHE:CE1 | 2.32                     | 0.55              |
| 41:BG:6:ALA:HB1    | 41:BG:105:LYS:NZ  | 2.21                     | 0.55              |
| 41:BG:71:THR:H     | 41:BG:90:LEU:H    | 1.54                     | 0.55              |
| 48:BP:33:ARG:O     | 48:BP:34:GLY:O    | 2.24                     | 0.55              |
| 51:BS:85:VAL:O     | 51:BS:106:ARG:HG2 | 2.06                     | 0.55              |
| 51:BS:83:LYS:O     | 51:BS:105:ALA:N   | 2.39                     | 0.55              |
| 52:BT:118:ARG:O    | 52:BT:119:LYS:HB2 | 2.07                     | 0.55              |
| 54:BV:18:LEU:HD22  | 54:BV:18:LEU:C    | 2.27                     | 0.55              |
| 58:BZ:129:SER:OG   | 58:BZ:132:ASN:HB3 | 2.07                     | 0.55              |
| 1:AA:774:G:C2'     | 1:AA:775:G:C5'    | 2.84                     | 0.55              |
| 4:AD:34:GLU:O      | 4:AD:35:ARG:CB    | 2.55                     | 0.55              |
| 7:AG:121:ALA:HA    | 7:AG:124:LEU:HB2  | 1.88                     | 0.55              |
| 10:AJ:28:ARG:C     | 10:AJ:30:SER:H    | 2.09                     | 0.55              |
| 16:AP:82:GLN:O     | 16:AP:84:ALA:N    | 2.39                     | 0.55              |
| 20:AT:72:LEU:O     | 20:AT:73:HIS:HB2  | 2.06                     | 0.55              |
| 24:AY:122:TRP:CH2  | 24:AY:132:ARG:HD2 | 2.41                     | 0.55              |
| 24:AY:469:GLU:HG2  | 24:AY:469:GLU:O   | 2.07                     | 0.55              |
| 24:AY:8:ASP:CB     | 24:AY:11:ARG:HD2  | 2.36                     | 0.55              |
| 29:B4:21:VAL:HG21  | 29:B4:35:VAL:HG23 | 1.88                     | 0.55              |
| 31:B6:5:VAL:O      | 31:B6:6:ARG:HB2   | 2.05                     | 0.55              |
| 33:B8:4:MET:CE     | 33:B8:61:LEU:HD23 | 2.36                     | 0.55              |
| 35:BA:1144:G:O2'   | 35:BA:1145:C:H5'  | 2.07                     | 0.55              |
| 35:BA:1377:G:H8    | 35:BA:1377:G:O5'  | 1.90                     | 0.55              |
| 35:BA:1877:A:H5'   | 35:BA:1878:G:OP2  | 2.07                     | 0.55              |
| 35:BA:1945:G:C5    | 35:BA:1946:U:C5   | 2.94                     | 0.55              |
| 35:BA:1983:C:O5'   | 35:BA:1983:C:H6   | 1.89                     | 0.55              |
| 35:BA:18:C:O2      | 35:BA:19:C:C6     | 2.60                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:363(F):A:H1' | 35:BA:364:C:H5     | 1.72                     | 0.55              |
| 35:BA:603:A:N7     | 35:BA:655:A:C6     | 2.74                     | 0.55              |
| 35:BA:655:A:C4'    | 35:BA:656:G:H5'    | 2.29                     | 0.55              |
| 35:BA:914:C:C2'    | 35:BA:915:C:H5'    | 2.30                     | 0.55              |
| 40:BF:125:LEU:HA   | 40:BF:194:MET:O    | 2.06                     | 0.55              |
| 35:BA:2849:U:P     | 52:BT:95:ARG:HH12  | 2.29                     | 0.55              |
| 53:BU:101:ARG:HG3  | 53:BU:101:ARG:NH1  | 2.20                     | 0.55              |
| 53:BU:92:ARG:HH11  | 53:BU:94:ASN:HD22  | 1.52                     | 0.55              |
| 54:BV:19:LYS:HG3   | 54:BV:20:LEU:N     | 2.22                     | 0.55              |
| 1:AA:560:U:C4'     | 1:AA:561:U:H5''    | 2.32                     | 0.55              |
| 8:AH:113:SER:HB2   | 8:AH:134:ILE:HD11  | 1.89                     | 0.55              |
| 9:AI:78:LYS:HD3    | 9:AI:79:LEU:N      | 2.21                     | 0.55              |
| 13:AM:84:ILE:HD12  | 19:AS:66:MET:SD    | 2.46                     | 0.55              |
| 24:AY:157:LEU:N    | 24:AY:157:LEU:HD23 | 2.21                     | 0.55              |
| 24:AY:232:LEU:HD12 | 45:BL:87:UNK:CB    | 2.36                     | 0.55              |
| 26:B1:86:SER:OG    | 26:B1:89:GLU:HG3   | 2.07                     | 0.55              |
| 29:B4:42:PHE:CE1   | 41:BG:180:PHE:CE1  | 2.95                     | 0.55              |
| 32:B7:34:ARG:HG3   | 32:B7:34:ARG:NH1   | 2.18                     | 0.55              |
| 35:BA:1144:G:H2'   | 35:BA:1145:C:C6    | 2.41                     | 0.55              |
| 35:BA:1385:G:H4'   | 35:BA:1386:C:OP1   | 2.05                     | 0.55              |
| 35:BA:1426:G:O5'   | 35:BA:1426:G:H8    | 1.90                     | 0.55              |
| 35:BA:858:U:O2     | 35:BA:2268:A:H2'   | 2.07                     | 0.55              |
| 35:BA:2523:G:H2'   | 35:BA:2524:G:C5'   | 2.36                     | 0.55              |
| 35:BA:39:C:HO2'    | 35:BA:40:C:H5'     | 1.67                     | 0.55              |
| 35:BA:47:C:N3      | 35:BA:179:G:N1     | 2.54                     | 0.55              |
| 35:BA:49:A:HO2'    | 35:BA:50:U:P       | 2.28                     | 0.55              |
| 35:BA:762:U:H4'    | 35:BA:763:G:O5'    | 2.06                     | 0.55              |
| 37:BC:121:MET:CA   | 37:BC:124:VAL:HG12 | 2.34                     | 0.55              |
| 38:BD:132:PRO:HG3  | 38:BD:190:TYR:CE1  | 2.42                     | 0.55              |
| 38:BD:35:LYS:HZ1   | 38:BD:35:LYS:HB3   | 1.72                     | 0.55              |
| 42:BH:106:THR:CG2  | 42:BH:112:PRO:HB3  | 2.29                     | 0.55              |
| 46:BN:133:GLN:O    | 46:BN:134:ARG:CB   | 2.54                     | 0.55              |
| 48:BP:115:LEU:N    | 48:BP:115:LEU:HD22 | 2.21                     | 0.55              |
| 56:BX:66:LEU:HD23  | 56:BX:66:LEU:O     | 2.06                     | 0.55              |
| 58:BZ:150:LEU:O    | 58:BZ:151:HIS:HB3  | 2.06                     | 0.55              |
| 58:BZ:48:PHE:HD1   | 58:BZ:48:PHE:O     | 1.90                     | 0.55              |
| 1:AA:1030:C:H4'    | 1:AA:1030(A):G:C5' | 2.36                     | 0.55              |
| 1:AA:1100:C:C5     | 2:AB:96:ARG:NH2    | 2.75                     | 0.55              |
| 1:AA:472:A:H2'     | 1:AA:473:G:O4'     | 2.07                     | 0.55              |
| 1:AA:555:C:N3      | 1:AA:556:C:N4      | 2.55                     | 0.55              |
| 1:AA:714:G:H2'     | 1:AA:715:A:C8      | 2.41                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:164:VAL:O     | 2:AB:186:ALA:CA    | 2.53                     | 0.55              |
| 2:AB:165:VAL:HG23  | 2:AB:166:ASP:N     | 2.22                     | 0.55              |
| 2:AB:71:VAL:CG1    | 2:AB:170:GLU:HG2   | 2.37                     | 0.55              |
| 3:AC:16:ARG:NH1    | 3:AC:16:ARG:HB2    | 2.20                     | 0.55              |
| 3:AC:25:GLY:C      | 3:AC:27:LYS:N      | 2.60                     | 0.55              |
| 11:AK:26:ASN:O     | 11:AK:27:ASN:HB2   | 2.06                     | 0.55              |
| 13:AM:3:ARG:N      | 13:AM:9:ILE:CG2    | 2.70                     | 0.55              |
| 24:AY:47:GLU:HB3   | 24:AY:52:MET:HB2   | 1.89                     | 0.55              |
| 27:B2:47:ASN:ND2   | 35:BA:94(A):G:N2   | 2.51                     | 0.55              |
| 30:B5:45:VAL:HG13  | 30:B5:51:TYR:CD1   | 2.42                     | 0.55              |
| 35:BA:1106:G:H2'   | 35:BA:1107:G:O4'   | 2.06                     | 0.55              |
| 35:BA:70:G:H2'     | 35:BA:113:G:O2'    | 2.06                     | 0.55              |
| 35:BA:1223:G:C2    | 35:BA:1227:G:C6    | 2.95                     | 0.55              |
| 35:BA:1416:G:C4    | 35:BA:1417:C:C4    | 2.95                     | 0.55              |
| 35:BA:1543:C:C3'   | 35:BA:1544:A:H5''  | 2.37                     | 0.55              |
| 35:BA:1599:C:H2'   | 35:BA:1600:C:C6    | 2.42                     | 0.55              |
| 35:BA:1845:G:O2'   | 35:BA:1846:G:H5'   | 2.06                     | 0.55              |
| 35:BA:188:G:H2'    | 35:BA:189:G:H5'    | 1.88                     | 0.55              |
| 35:BA:1971:A:H1'   | 38:BD:240:ALA:O    | 2.07                     | 0.55              |
| 35:BA:2136:C:H2'   | 35:BA:2137:C:C6    | 2.42                     | 0.55              |
| 35:BA:2111:C:C2    | 35:BA:2147:G:N2    | 2.74                     | 0.55              |
| 35:BA:2360:A:O2'   | 35:BA:2361:A:H8    | 1.89                     | 0.55              |
| 35:BA:2581:G:C2'   | 35:BA:2610:C:N4    | 2.68                     | 0.55              |
| 36:BB:17:C:O2'     | 36:BB:18:G:H5'     | 2.06                     | 0.55              |
| 36:BB:24:G:H4'     | 36:BB:25:A:C8      | 2.42                     | 0.55              |
| 37:BC:52:PRO:HB2   | 37:BC:168:LYS:O    | 2.07                     | 0.55              |
| 39:BE:104:VAL:HG22 | 39:BE:198:VAL:HG13 | 1.88                     | 0.55              |
| 39:BE:120:TRP:O    | 39:BE:121:ASN:C    | 2.45                     | 0.55              |
| 41:BG:133:LEU:CD1  | 41:BG:134:GLY:N    | 2.70                     | 0.55              |
| 48:BP:23:PRO:CB    | 48:BP:33:ARG:HG2   | 2.37                     | 0.55              |
| 51:BS:89:ARG:HH11  | 51:BS:89:ARG:HG2   | 1.72                     | 0.55              |
| 52:BT:16:ARG:HG3   | 52:BT:79:HIS:HA    | 1.88                     | 0.55              |
| 52:BT:90:GLN:O     | 52:BT:92:GLY:N     | 2.40                     | 0.55              |
| 53:BU:84:LYS:CD    | 53:BU:89:GLU:HG3   | 2.37                     | 0.55              |
| 54:BV:51:VAL:HG12  | 54:BV:52:VAL:H     | 1.72                     | 0.55              |
| 58:BZ:43:GLU:O     | 58:BZ:47:VAL:HG23  | 2.07                     | 0.55              |
| 1:AA:1071:C:H2'    | 1:AA:1072:G:C8     | 2.41                     | 0.55              |
| 1:AA:1081:G:O2'    | 1:AA:1082:G:H5'    | 2.07                     | 0.55              |
| 1:AA:187:C:H2'     | 1:AA:188:C:H6      | 1.72                     | 0.55              |
| 1:AA:187:C:H2'     | 1:AA:188:C:C6      | 2.41                     | 0.55              |
| 1:AA:688:G:N2      | 1:AA:699:C:O2      | 2.36                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:775:G:H2'     | 1:AA:776:G:H5'     | 1.87                     | 0.55              |
| 1:AA:795:C:H6      | 1:AA:795:C:O5'     | 1.90                     | 0.55              |
| 3:AC:11:ARG:HB3    | 3:AC:15:THR:HB     | 1.89                     | 0.55              |
| 14:AN:7:ILE:HG13   | 14:AN:8:GLU:HG3    | 1.88                     | 0.55              |
| 1:AA:191:G:H1'     | 20:AT:105:SER:HA   | 1.87                     | 0.55              |
| 22:AV:41:C:HO2'    | 22:AV:42:C:H5'     | 1.67                     | 0.55              |
| 24:AY:264:LEU:HD12 | 61:AY:701:GCP:C2   | 2.37                     | 0.55              |
| 24:AY:309:LEU:HB3  | 24:AY:391:GLY:N    | 2.22                     | 0.55              |
| 24:AY:556:ILE:HD13 | 24:AY:601:ILE:HD13 | 1.89                     | 0.55              |
| 25:B0:10:THR:C     | 25:B0:11:ARG:CG    | 2.75                     | 0.55              |
| 31:B6:26:ASN:HD21  | 31:B6:32:ASN:ND2   | 2.05                     | 0.55              |
| 31:B6:44:ARG:C     | 31:B6:45:LYS:HG2   | 2.27                     | 0.55              |
| 35:BA:1021:A:H61   | 35:BA:1142(A):A:N6 | 2.04                     | 0.55              |
| 35:BA:1649:G:HO2'  | 35:BA:1650:G:H5'   | 1.68                     | 0.55              |
| 35:BA:1827:C:C2'   | 35:BA:1828:G:H5'   | 2.36                     | 0.55              |
| 35:BA:747:U:H5     | 35:BA:2014:A:N3    | 2.04                     | 0.55              |
| 35:BA:2126:A:O2'   | 35:BA:2127:G:C5'   | 2.54                     | 0.55              |
| 35:BA:2757:A:H2'   | 35:BA:2758:A:O5'   | 2.06                     | 0.55              |
| 35:BA:363(F):A:H4' | 35:BA:364:C:O5'    | 2.07                     | 0.55              |
| 35:BA:28:A:N6      | 35:BA:512:G:H1'    | 2.21                     | 0.55              |
| 35:BA:573:G:O2'    | 35:BA:574:C:H3'    | 2.07                     | 0.55              |
| 35:BA:637:A:N1     | 35:BA:652:C:H5'    | 2.22                     | 0.55              |
| 35:BA:858:U:O2'    | 35:BA:859:G:C4     | 2.60                     | 0.55              |
| 38:BD:218:ARG:HB3  | 38:BD:219:PRO:HD2  | 1.88                     | 0.55              |
| 40:BF:184:TYR:O    | 40:BF:188:ARG:HG2  | 2.07                     | 0.55              |
| 41:BG:7:LEU:HB2    | 41:BG:104:GLU:HG3  | 1.88                     | 0.55              |
| 51:BS:12:PHE:O     | 51:BS:14:VAL:HG23  | 2.07                     | 0.55              |
| 52:BT:25:GLY:HA2   | 52:BT:92:GLY:HA2   | 1.89                     | 0.55              |
| 53:BU:17:ILE:HA    | 53:BU:20:LEU:HD23  | 1.88                     | 0.55              |
| 54:BV:21:ARG:HG2   | 54:BV:91:TYR:CD1   | 2.42                     | 0.55              |
| 1:AA:490:G:C5      | 1:AA:491:G:N7      | 2.74                     | 0.55              |
| 1:AA:561:U:C6      | 1:AA:561:U:OP1     | 2.59                     | 0.55              |
| 1:AA:751:U:O2'     | 1:AA:752:G:H5'     | 2.06                     | 0.55              |
| 1:AA:862:C:O2'     | 1:AA:863:U:C5'     | 2.55                     | 0.55              |
| 1:AA:936:C:H2'     | 1:AA:937:A:C5'     | 2.37                     | 0.55              |
| 1:AA:996:A:H2'     | 1:AA:997:U:C6      | 2.42                     | 0.55              |
| 3:AC:113:ALA:HB3   | 3:AC:114:PRO:HD3   | 1.87                     | 0.55              |
| 3:AC:131:ARG:HD3   | 3:AC:166:GLU:HG2   | 1.89                     | 0.55              |
| 6:AF:28:ARG:HG3    | 6:AF:28:ARG:NH1    | 2.21                     | 0.55              |
| 16:AP:75:ARG:HH11  | 16:AP:75:ARG:HG3   | 1.72                     | 0.55              |
| 24:AY:192:LEU:HD12 | 24:AY:194:THR:HG23 | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:AY:505:GLY:O   | 24:AY:506:GLN:HG3 | 2.07                     | 0.55              |
| 26:B1:37:ILE:HD12 | 26:B1:38:SER:N    | 2.22                     | 0.55              |
| 35:BA:1050:A:H2'  | 35:BA:1051:G:C8   | 2.41                     | 0.55              |
| 35:BA:1301:A:HO2' | 35:BA:1302:A:P    | 2.30                     | 0.55              |
| 35:BA:1684:C:H2'  | 35:BA:1685:C:C6   | 2.42                     | 0.55              |
| 35:BA:175:G:H2'   | 35:BA:176:G:H5'   | 1.88                     | 0.55              |
| 35:BA:2448:A:HO2' | 35:BA:2449:U:H5   | 1.54                     | 0.55              |
| 34:B9:31:LYS:HE2  | 35:BA:2478:A:H5'  | 1.87                     | 0.55              |
| 35:BA:541:C:O2'   | 35:BA:542:C:H5'   | 2.07                     | 0.55              |
| 40:BF:64:ILE:HD12 | 40:BF:78:ILE:CG2  | 2.37                     | 0.55              |
| 41:BG:41:GLN:HG3  | 41:BG:154:GLY:O   | 2.07                     | 0.55              |
| 43:BJ:22:UNK:O    | 43:BJ:118:UNK:HA  | 2.06                     | 0.55              |
| 52:BT:126:ALA:O   | 52:BT:128:GLU:N   | 2.39                     | 0.55              |
| 57:BY:13:VAL:HG23 | 57:BY:73:ARG:C    | 2.28                     | 0.55              |
| 57:BY:76:CYS:SG   | 57:BY:77:PRO:CD   | 2.77                     | 0.55              |
| 1:AA:1281:U:P     | 1:AA:1282:C:H41   | 2.30                     | 0.55              |
| 1:AA:1329:A:P     | 13:AM:28:ALA:HB3  | 2.47                     | 0.55              |
| 1:AA:1499:A:N3    | 1:AA:1500:A:C8    | 2.75                     | 0.55              |
| 1:AA:163:C:H2'    | 1:AA:164:U:H6     | 1.70                     | 0.55              |
| 1:AA:184:G:O2'    | 1:AA:185:A:H5'    | 2.06                     | 0.55              |
| 1:AA:21:G:H2'     | 1:AA:22:G:C8      | 2.41                     | 0.55              |
| 1:AA:495:A:O2'    | 1:AA:496:A:C3'    | 2.55                     | 0.55              |
| 1:AA:828:A:H2'    | 1:AA:829:G:O4'    | 2.07                     | 0.55              |
| 1:AA:848:C:H2'    | 1:AA:849:C:H6     | 1.71                     | 0.55              |
| 4:AD:173:TRP:HB2  | 4:AD:187:ARG:O    | 2.06                     | 0.55              |
| 7:AG:131:LYS:H    | 7:AG:131:LYS:HD2  | 1.71                     | 0.55              |
| 7:AG:69:VAL:HG21  | 7:AG:134:ALA:HB1  | 1.89                     | 0.55              |
| 3:AC:13:GLY:HA3   | 14:AN:57:ARG:NH1  | 2.22                     | 0.55              |
| 19:AS:22:LEU:O    | 19:AS:26:GLY:N    | 2.40                     | 0.55              |
| 24:AY:36:THR:O    | 24:AY:38:ARG:N    | 2.40                     | 0.55              |
| 24:AY:454:MET:N   | 24:AY:458:HIS:HD2 | 1.90                     | 0.55              |
| 31:B6:15:GLU:CG   | 31:B6:18:ARG:NH1  | 2.70                     | 0.55              |
| 34:B9:4:ARG:O     | 34:B9:36:GLN:HA   | 2.07                     | 0.55              |
| 35:BA:1445:A:H8   | 35:BA:1460:A:C2   | 2.18                     | 0.55              |
| 35:BA:1658:C:OP1  | 39:BE:132:HIS:CE1 | 2.60                     | 0.55              |
| 35:BA:2115:G:H5'  | 35:BA:2116:G:OP2  | 2.07                     | 0.55              |
| 35:BA:968:G:C2'   | 35:BA:969:U:H5'   | 2.33                     | 0.55              |
| 36:BB:28:C:H2'    | 36:BB:29:A:C8     | 2.42                     | 0.55              |
| 38:BD:148:GLU:HB2 | 38:BD:151:LYS:HD2 | 1.89                     | 0.55              |
| 35:BA:1902:C:H1'  | 38:BD:244:ARG:HG3 | 1.89                     | 0.55              |
| 42:BH:10:PRO:HB2  | 42:BH:49:VAL:CG1  | 2.36                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:BO:87:ILE:HG23 | 47:BO:91:LEU:HA   | 1.88                     | 0.55              |
| 51:BS:96:GLY:C    | 51:BS:98:VAL:H    | 2.10                     | 0.55              |
| 35:BA:81:G:H21    | 57:BY:2:ARG:CZ    | 2.20                     | 0.55              |
| 58:BZ:81:ARG:NH1  | 58:BZ:81:ARG:HB2  | 2.22                     | 0.55              |
| 1:AA:1051:C:O5'   | 1:AA:1051:C:H6    | 1.90                     | 0.54              |
| 1:AA:1216:G:H5''  | 14:AN:5:ALA:HB2   | 1.89                     | 0.54              |
| 1:AA:298:A:H2'    | 1:AA:299:G:O4'    | 2.08                     | 0.54              |
| 1:AA:859:A:H2'    | 1:AA:860:A:C5'    | 2.34                     | 0.54              |
| 1:AA:875:C:H1'    | 8:AH:15:ASN:OD1   | 2.07                     | 0.54              |
| 4:AD:70:ILE:HD11  | 4:AD:100:ARG:HD2  | 1.89                     | 0.54              |
| 9:AI:59:PHE:HZ    | 9:AI:88:TYR:CE2   | 2.25                     | 0.54              |
| 22:AV:45:U:O2     | 22:AV:45:U:H3'    | 2.07                     | 0.54              |
| 24:AY:99:ARG:HH22 | 24:AY:403:GLU:HB2 | 1.70                     | 0.54              |
| 24:AY:490:PRO:HG3 | 24:AY:516:PRO:HD2 | 1.89                     | 0.54              |
| 25:B0:45:PHE:HZ   | 25:B0:77:ARG:NH2  | 2.04                     | 0.54              |
| 27:B2:10:LEU:O    | 27:B2:14:ARG:CB   | 2.50                     | 0.54              |
| 31:B6:13:CYS:O    | 31:B6:21:TYR:HA   | 2.07                     | 0.54              |
| 33:B8:13:ARG:NH2  | 35:BA:250:G:OP2   | 2.40                     | 0.54              |
| 35:BA:1168:G:O2'  | 35:BA:1169:G:H5'  | 2.07                     | 0.54              |
| 35:BA:2466:C:O2'  | 35:BA:2467:C:H5'  | 2.07                     | 0.54              |
| 35:BA:2481:G:O2'  | 35:BA:2482:G:P    | 2.65                     | 0.54              |
| 35:BA:248:G:C2'   | 35:BA:249:C:OP1   | 2.55                     | 0.54              |
| 35:BA:35:G:C6     | 35:BA:446:G:N2    | 2.75                     | 0.54              |
| 35:BA:536:A:H2'   | 35:BA:537:C:C6    | 2.42                     | 0.54              |
| 35:BA:603:A:C1'   | 35:BA:604:G:P     | 2.96                     | 0.54              |
| 35:BA:831:G:O3'   | 48:BP:40:SER:CB   | 2.56                     | 0.54              |
| 35:BA:856:C:HO2'  | 35:BA:857:C:P     | 2.30                     | 0.54              |
| 38:BD:210:GLY:O   | 38:BD:211:ARG:CB  | 2.53                     | 0.54              |
| 39:BE:132:HIS:C   | 39:BE:135:HIS:NE2 | 2.60                     | 0.54              |
| 39:BE:71:GLY:C    | 39:BE:73:GLU:H    | 2.10                     | 0.54              |
| 41:BG:104:GLU:CB  | 41:BG:105:LYS:HE2 | 2.37                     | 0.54              |
| 42:BH:81:GLU:HG2  | 42:BH:83:TYR:OH   | 2.07                     | 0.54              |
| 44:BK:131:UNK:O   | 44:BK:132:UNK:C   | 2.54                     | 0.54              |
| 51:BS:15:ARG:NH1  | 51:BS:15:ARG:CB   | 2.70                     | 0.54              |
| 52:BT:106:SER:O   | 52:BT:107:ASP:CB  | 2.54                     | 0.54              |
| 53:BU:84:LYS:HD3  | 53:BU:89:GLU:HG3  | 1.89                     | 0.54              |
| 54:BV:79:VAL:CG1  | 54:BV:79:VAL:O    | 2.54                     | 0.54              |
| 57:BY:3:VAL:H     | 57:BY:5:MET:CE    | 2.20                     | 0.54              |
| 1:AA:348:G:C2     | 1:AA:349:A:C8     | 2.94                     | 0.54              |
| 1:AA:368:U:H3'    | 1:AA:368:U:H6     | 1.73                     | 0.54              |
| 1:AA:792:A:H4'    | 1:AA:793:U:C5'    | 2.37                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:132:LYS:HA   | 2:AB:135:GLN:CG   | 2.37                     | 0.54              |
| 3:AC:187:ALA:O    | 3:AC:188:LEU:HB2  | 2.07                     | 0.54              |
| 3:AC:43:LEU:HD22  | 3:AC:47:LEU:HD22  | 1.90                     | 0.54              |
| 4:AD:61:LYS:HA    | 4:AD:203:VAL:HG22 | 1.89                     | 0.54              |
| 7:AG:50:ILE:CG2   | 7:AG:58:PRO:HG3   | 2.37                     | 0.54              |
| 7:AG:89:MET:HG3   | 7:AG:90:GLU:OE2   | 2.08                     | 0.54              |
| 8:AH:110:ALA:HB3  | 8:AH:121:ASP:HB3  | 1.89                     | 0.54              |
| 10:AJ:22:LYS:CD   | 10:AJ:90:LEU:HD22 | 2.37                     | 0.54              |
| 13:AM:10:PRO:HB2  | 13:AM:18:ALA:CB   | 2.37                     | 0.54              |
| 13:AM:4:ILE:CG2   | 13:AM:5:ALA:N     | 2.58                     | 0.54              |
| 19:AS:22:LEU:O    | 19:AS:22:LEU:HD13 | 2.06                     | 0.54              |
| 22:AV:40:C:C2'    | 22:AV:41:C:H5'    | 2.36                     | 0.54              |
| 24:AY:156:ARG:NH2 | 24:AY:666:ARG:NH1 | 2.55                     | 0.54              |
| 24:AY:30:GLU:HB2  | 24:AY:52:MET:HE2  | 1.89                     | 0.54              |
| 29:B4:64:GLY:HA3  | 29:B4:67:TYR:CE2  | 2.42                     | 0.54              |
| 31:B6:15:GLU:HG2  | 31:B6:18:ARG:NH1  | 2.22                     | 0.54              |
| 35:BA:109:G:C2'   | 35:BA:110:G:O5'   | 2.55                     | 0.54              |
| 35:BA:1313:U:H2'  | 35:BA:1610:A:N1   | 2.21                     | 0.54              |
| 35:BA:15:G:HO2'   | 35:BA:16:G:H5'    | 1.69                     | 0.54              |
| 35:BA:1722:A:C2   | 35:BA:1740:G:H2'  | 2.42                     | 0.54              |
| 35:BA:2403:C:C2'  | 35:BA:2404:C:H5'  | 2.37                     | 0.54              |
| 35:BA:2409:G:HO2' | 35:BA:2410:G:H5'  | 1.71                     | 0.54              |
| 35:BA:29:U:HO2'   | 35:BA:30:G:H5'    | 1.70                     | 0.54              |
| 35:BA:433:C:H2'   | 35:BA:434:U:C6    | 2.42                     | 0.54              |
| 38:BD:186:HIS:HD2 | 38:BD:188:GLU:HB2 | 1.72                     | 0.54              |
| 35:BA:1813:G:H1'  | 38:BD:50:THR:OG1  | 2.06                     | 0.54              |
| 39:BE:141:ILE:C   | 39:BE:154:LYS:HE2 | 2.26                     | 0.54              |
| 41:BG:108:ASN:O   | 41:BG:109:VAL:HB  | 2.07                     | 0.54              |
| 51:BS:30:ARG:NH1  | 51:BS:97:ARG:HG2  | 2.19                     | 0.54              |
| 52:BT:92:GLY:HA3  | 52:BT:120:ARG:NH2 | 2.22                     | 0.54              |
| 52:BT:30:VAL:HG13 | 52:BT:84:GLN:O    | 2.07                     | 0.54              |
| 1:AA:1048:G:C2    | 1:AA:1050:G:N7    | 2.75                     | 0.54              |
| 1:AA:1351:U:H4'   | 7:AG:33:ASP:OD2   | 2.07                     | 0.54              |
| 1:AA:1372:U:H2'   | 1:AA:1373:G:O4'   | 2.07                     | 0.54              |
| 1:AA:266:G:O2'    | 1:AA:267:C:P      | 2.66                     | 0.54              |
| 1:AA:40:C:O2'     | 1:AA:41:G:C5'     | 2.53                     | 0.54              |
| 2:AB:104:ASN:ND2  | 2:AB:107:THR:HB   | 2.22                     | 0.54              |
| 2:AB:223:ILE:CG2  | 2:AB:227:GLY:O    | 2.50                     | 0.54              |
| 6:AF:20:ALA:O     | 6:AF:24:GLU:HB2   | 2.07                     | 0.54              |
| 9:AI:18:PHE:O     | 9:AI:62:TYR:N     | 2.41                     | 0.54              |
| 9:AI:26:VAL:HG13  | 9:AI:27:THR:N     | 2.21                     | 0.54              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 20:AT:99:LEU:O      | 20:AT:100:ILE:C   | 2.46                     | 0.54              |
| 31:B6:25:LYS:CE     | 33:B8:34:TRP:HE1  | 2.18                     | 0.54              |
| 35:BA:1092:C:H2'    | 35:BA:1093:G:O4'  | 2.07                     | 0.54              |
| 35:BA:54:G:O6       | 35:BA:117:G:N2    | 2.40                     | 0.54              |
| 35:BA:1541:G:O2'    | 35:BA:1542:A:H5'' | 2.08                     | 0.54              |
| 35:BA:1995:U:H2'    | 35:BA:1996:C:C5   | 2.42                     | 0.54              |
| 35:BA:2203:U:H1'    | 35:BA:2221:G:N2   | 2.23                     | 0.54              |
| 35:BA:2894:G:N3     | 35:BA:2894:G:H2'  | 2.23                     | 0.54              |
| 35:BA:654(G):C:HO2' | 35:BA:654(H):G:H8 | 1.55                     | 0.54              |
| 35:BA:718:A:H2'     | 35:BA:719:C:O4'   | 2.06                     | 0.54              |
| 35:BA:858:U:O2'     | 35:BA:859:G:C5    | 2.60                     | 0.54              |
| 35:BA:942:G:O2'     | 35:BA:943:U:H5'   | 2.06                     | 0.54              |
| 37:BC:6:LYS:HA      | 37:BC:9:ARG:HH11  | 1.72                     | 0.54              |
| 37:BC:88:GLU:HG3    | 37:BC:89:GLU:N    | 2.22                     | 0.54              |
| 47:BO:68:GLU:HB3    | 47:BO:78:ARG:HD3  | 1.90                     | 0.54              |
| 48:BP:115:LEU:CD2   | 48:BP:115:LEU:N   | 2.70                     | 0.54              |
| 51:BS:28:VAL:CG1    | 51:BS:29:PHE:H    | 2.19                     | 0.54              |
| 51:BS:66:ALA:CA     | 51:BS:69:VAL:HG12 | 2.33                     | 0.54              |
| 1:AA:106:C:H2'      | 1:AA:107:G:C8     | 2.36                     | 0.54              |
| 1:AA:113:G:O4'      | 1:AA:354:G:H4'    | 2.06                     | 0.54              |
| 1:AA:47:C:OP2       | 1:AA:366:C:N4     | 2.36                     | 0.54              |
| 1:AA:690:G:O6       | 1:AA:691:G:C6     | 2.61                     | 0.54              |
| 1:AA:773:G:N3       | 1:AA:774:G:C8     | 2.76                     | 0.54              |
| 2:AB:167:PRO:HG2    | 2:AB:192:SER:HB2  | 1.90                     | 0.54              |
| 2:AB:185:ILE:HG23   | 2:AB:199:TYR:CB   | 2.36                     | 0.54              |
| 10:AJ:87:THR:OG1    | 10:AJ:88:LEU:N    | 2.40                     | 0.54              |
| 11:AK:20:TYR:C      | 11:AK:21:ILE:HD12 | 2.28                     | 0.54              |
| 12:AL:24:VAL:HG13   | 12:AL:98:TYR:CE2  | 2.40                     | 0.54              |
| 19:AS:39:THR:HA     | 19:AS:70:LYS:HD3  | 1.90                     | 0.54              |
| 20:AT:36:LEU:CD1    | 20:AT:55:ILE:HG23 | 2.37                     | 0.54              |
| 26:B1:19:GLN:O      | 26:B1:35:THR:HG22 | 2.06                     | 0.54              |
| 27:B2:47:ASN:O      | 27:B2:50:ILE:N    | 2.41                     | 0.54              |
| 19:AS:20:LEU:HD13   | 29:B4:61:ARG:HH21 | 1.73                     | 0.54              |
| 31:B6:15:GLU:HG2    | 31:B6:18:ARG:HD3  | 1.89                     | 0.54              |
| 33:B8:53:PRO:HA     | 33:B8:56:GLU:HB2  | 1.88                     | 0.54              |
| 35:BA:1416:G:C2     | 35:BA:1417:C:C4   | 2.95                     | 0.54              |
| 35:BA:2101:G:H2'    | 35:BA:2102:U:O4'  | 2.08                     | 0.54              |
| 35:BA:654(A):G:H1   | 35:BA:654(S):G:N2 | 2.05                     | 0.54              |
| 25:B0:26:TYR:CD2    | 35:BA:857:C:H1'   | 2.42                     | 0.54              |
| 37:BC:117:THR:HG23  | 37:BC:119:ASP:OD1 | 2.07                     | 0.54              |
| 35:BA:2579:C:O2'    | 39:BE:131:ALA:HB3 | 2.07                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BE:69:LYS:C     | 39:BE:71:GLY:N     | 2.58                     | 0.54              |
| 41:BG:141:PHE:HA   | 41:BG:142:PRO:O    | 2.08                     | 0.54              |
| 42:BH:86:GLU:HA    | 42:BH:132:ARG:HA   | 1.88                     | 0.54              |
| 51:BS:14:VAL:HG12  | 51:BS:15:ARG:H     | 1.72                     | 0.54              |
| 58:BZ:60:GLU:O     | 58:BZ:61:LEU:HG    | 2.08                     | 0.54              |
| 1:AA:1250:A:H4'    | 9:AI:68:GLY:N      | 2.20                     | 0.54              |
| 1:AA:1352:C:H2'    | 1:AA:1353:G:C8     | 2.43                     | 0.54              |
| 1:AA:1387:G:H2'    | 1:AA:1388:C:C6     | 2.43                     | 0.54              |
| 1:AA:346:G:H2'     | 1:AA:346:G:N3      | 2.22                     | 0.54              |
| 1:AA:867:G:H2'     | 1:AA:868:C:H5'     | 1.89                     | 0.54              |
| 2:AB:167:PRO:CG    | 2:AB:188:ALA:CB    | 2.86                     | 0.54              |
| 2:AB:35:GLU:HG2    | 2:AB:35:GLU:O      | 2.07                     | 0.54              |
| 5:AE:47:LYS:O      | 5:AE:57:LYS:HE3    | 2.06                     | 0.54              |
| 11:AK:22:HIS:HB3   | 11:AK:29:ILE:HG23  | 1.89                     | 0.54              |
| 14:AN:7:ILE:HG13   | 14:AN:8:GLU:N      | 2.23                     | 0.54              |
| 15:AO:17:ARG:NH1   | 15:AO:77:ARG:NH1   | 2.55                     | 0.54              |
| 19:AS:35:SER:C     | 19:AS:37:ARG:H     | 2.09                     | 0.54              |
| 25:B0:36:ILE:HD11  | 35:BA:2355:C:O4'   | 2.08                     | 0.54              |
| 27:B2:47:ASN:O     | 27:B2:48:HIS:C     | 2.45                     | 0.54              |
| 28:B3:7:LYS:HB2    | 28:B3:34:GLU:HB3   | 1.90                     | 0.54              |
| 30:B5:37:LYS:HG3   | 30:B5:37:LYS:O     | 2.07                     | 0.54              |
| 35:BA:1092:C:C2'   | 35:BA:1093:G:H5'   | 2.38                     | 0.54              |
| 28:B3:29:ARG:NH1   | 35:BA:1183:G:O3'   | 2.37                     | 0.54              |
| 35:BA:1382:G:H2'   | 35:BA:1383:C:C6    | 2.43                     | 0.54              |
| 35:BA:1982:C:N3    | 35:BA:1983:C:C4    | 2.76                     | 0.54              |
| 35:BA:272(H):C:H2' | 35:BA:272(I):U:C5' | 2.37                     | 0.54              |
| 35:BA:794:G:H2'    | 35:BA:795:C:C6     | 2.43                     | 0.54              |
| 37:BC:30:VAL:HG23  | 37:BC:31:LYS:HG2   | 1.89                     | 0.54              |
| 37:BC:44:VAL:HG23  | 37:BC:176:VAL:HG21 | 1.89                     | 0.54              |
| 38:BD:79:VAL:CG2   | 38:BD:111:LEU:HD11 | 2.37                     | 0.54              |
| 39:BE:21:VAL:O     | 39:BE:23:VAL:HG13  | 2.07                     | 0.54              |
| 40:BF:133:ASN:HA   | 40:BF:162:LEU:HD23 | 1.88                     | 0.54              |
| 40:BF:20:LEU:N     | 40:BF:24:LEU:CD2   | 2.69                     | 0.54              |
| 46:BN:67:LEU:HB3   | 46:BN:88:GLU:HG2   | 1.88                     | 0.54              |
| 50:BR:7:GLY:CA     | 50:BR:8:ARG:NH2    | 2.67                     | 0.54              |
| 54:BV:25:LEU:H     | 54:BV:92:THR:CG2   | 2.20                     | 0.54              |
| 53:BU:90:VAL:HG21  | 54:BV:47:VAL:HG21  | 1.90                     | 0.54              |
| 1:AA:1035:A:H2'    | 1:AA:1036:G:O4'    | 2.08                     | 0.54              |
| 1:AA:1089:G:HO2'   | 1:AA:1170:A:H2     | 1.55                     | 0.54              |
| 1:AA:1256:A:H2     | 1:AA:1277:C:N3     | 2.06                     | 0.54              |
| 1:AA:690:G:C6      | 1:AA:691:G:N1      | 2.76                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:773:G:N2      | 1:AA:774:G:C4      | 2.76                     | 0.54              |
| 2:AB:16:HIS:O      | 2:AB:17:PHE:CB     | 2.54                     | 0.54              |
| 2:AB:89:GLY:C      | 2:AB:90:MET:CG     | 2.75                     | 0.54              |
| 3:AC:130:VAL:O     | 3:AC:130:VAL:HG12  | 2.07                     | 0.54              |
| 1:AA:427:U:OP1     | 4:AD:13:ARG:NH2    | 2.41                     | 0.54              |
| 13:AM:20:THR:HA    | 13:AM:25:ILE:O     | 2.08                     | 0.54              |
| 13:AM:45:VAL:C     | 13:AM:47:ASP:H     | 2.11                     | 0.54              |
| 10:AJ:53:PRO:HA    | 14:AN:42:ILE:CD1   | 2.37                     | 0.54              |
| 24:AY:122:TRP:CZ3  | 24:AY:132:ARG:HD2  | 2.42                     | 0.54              |
| 28:B3:31:LEU:O     | 28:B3:33:GLN:N     | 2.31                     | 0.54              |
| 33:B8:4:MET:HB3    | 33:B8:61:LEU:HD22  | 1.89                     | 0.54              |
| 35:BA:1516:C:C2'   | 35:BA:1517:G:C5'   | 2.86                     | 0.54              |
| 35:BA:963:U:H2'    | 35:BA:964:C:C6     | 2.43                     | 0.54              |
| 37:BC:49:GLY:N     | 37:BC:209:PHE:O    | 2.39                     | 0.54              |
| 37:BC:194:ILE:HD11 | 37:BC:227:PRO:HB3  | 1.89                     | 0.54              |
| 39:BE:53:PRO:C     | 39:BE:54:GLN:HG2   | 2.28                     | 0.54              |
| 42:BH:11:VAL:HG13  | 42:BH:15:VAL:CG2   | 2.38                     | 0.54              |
| 46:BN:99:LEU:HD13  | 46:BN:99:LEU:O     | 2.08                     | 0.54              |
| 47:BO:7:TYR:CZ     | 47:BO:44:LYS:HG3   | 2.42                     | 0.54              |
| 48:BP:114:ILE:HD12 | 48:BP:114:ILE:O    | 2.08                     | 0.54              |
| 50:BR:88:ARG:O     | 50:BR:88:ARG:HD2   | 2.07                     | 0.54              |
| 52:BT:23:ARG:CB    | 52:BT:24:PRO:HD3   | 2.35                     | 0.54              |
| 53:BU:34:LYS:CA    | 53:BU:34:LYS:HE2   | 2.30                     | 0.54              |
| 53:BU:52:ARG:HH11  | 53:BU:52:ARG:HB3   | 1.71                     | 0.54              |
| 54:BV:72:VAL:CG2   | 54:BV:85:LYS:HB3   | 2.38                     | 0.54              |
| 35:BA:484:C:OP1    | 57:BY:49:VAL:HG13  | 2.07                     | 0.54              |
| 1:AA:1228:C:H4'    | 13:AM:116:THR:O    | 2.07                     | 0.54              |
| 1:AA:1306:A:N6     | 1:AA:1331:G:C2'    | 2.70                     | 0.54              |
| 1:AA:1323:G:H2'    | 1:AA:1324:A:C8     | 2.43                     | 0.54              |
| 1:AA:1384:C:N3     | 1:AA:1385:G:N7     | 2.56                     | 0.54              |
| 1:AA:1400:C:N4     | 22:AV:34:G:C8      | 2.76                     | 0.54              |
| 1:AA:235:C:C5'     | 17:AQ:70:ARG:HG2   | 2.37                     | 0.54              |
| 1:AA:561:U:H6      | 1:AA:561:U:OP1     | 1.91                     | 0.54              |
| 1:AA:687:A:C1'     | 1:AA:688:G:P       | 2.96                     | 0.54              |
| 2:AB:10:LEU:O      | 2:AB:10:LEU:HD23   | 2.07                     | 0.54              |
| 7:AG:70:LYS:HB3    | 7:AG:100:ALA:HB2   | 1.89                     | 0.54              |
| 12:AL:17:LYS:NZ    | 12:AL:18:VAL:HG22  | 2.23                     | 0.54              |
| 12:AL:28:LYS:HE3   | 12:AL:33:ARG:HH12  | 1.73                     | 0.54              |
| 13:AM:108:ARG:CG   | 13:AM:108:ARG:HH11 | 2.19                     | 0.54              |
| 13:AM:13:LYS:O     | 13:AM:45:VAL:HG23  | 2.08                     | 0.54              |
| 1:AA:1314:C:C5     | 19:AS:6:LYS:NZ     | 2.75                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:25:LYS:NZ    | 24:AY:86:GLY:HA3   | 2.22                     | 0.54              |
| 24:AY:312:LEU:HD11 | 24:AY:401:SER:CB   | 2.36                     | 0.54              |
| 24:AY:573:HIS:CG   | 24:AY:573:HIS:O    | 2.60                     | 0.54              |
| 24:AY:614:GLU:HA   | 24:AY:617:MET:CE   | 2.37                     | 0.54              |
| 31:B6:12:GLU:HB3   | 31:B6:23:THR:HG22  | 1.89                     | 0.54              |
| 35:BA:1071:G:H1'   | 35:BA:1089:G:C8    | 2.43                     | 0.54              |
| 35:BA:1595:G:C2'   | 35:BA:1596:A:H5'   | 2.37                     | 0.54              |
| 35:BA:2062:A:H5'   | 35:BA:2062:A:C8    | 2.43                     | 0.54              |
| 35:BA:2404:C:C4    | 35:BA:2414:G:N1    | 2.75                     | 0.54              |
| 35:BA:2523:G:H2'   | 35:BA:2524:G:H5''  | 1.88                     | 0.54              |
| 35:BA:26:G:C6      | 35:BA:27:G:N1      | 2.75                     | 0.54              |
| 35:BA:653:A:C3'    | 35:BA:653:A:N3     | 2.66                     | 0.54              |
| 35:BA:706:A:H2'    | 35:BA:707:G:O4'    | 2.08                     | 0.54              |
| 37:BC:72:GLN:HA    | 37:BC:72:GLN:NE2   | 2.23                     | 0.54              |
| 39:BE:141:ILE:O    | 39:BE:154:LYS:HE2  | 2.07                     | 0.54              |
| 40:BF:102:PRO:HB2  | 40:BF:105:VAL:HG23 | 1.89                     | 0.54              |
| 40:BF:3:GLU:C      | 40:BF:24:LEU:HG    | 2.26                     | 0.54              |
| 42:BH:85:LYS:O     | 42:BH:85:LYS:HD3   | 2.07                     | 0.54              |
| 46:BN:73:THR:HG23  | 46:BN:82:LEU:HD11  | 1.90                     | 0.54              |
| 53:BU:8:VAL:HG23   | 53:BU:11:ARG:HH21  | 1.73                     | 0.54              |
| 58:BZ:6:LYS:N      | 58:BZ:6:LYS:HD3    | 2.23                     | 0.54              |
| 1:AA:1137:C:H4'    | 1:AA:1138:G:N2     | 2.22                     | 0.54              |
| 1:AA:1228:C:OP1    | 13:AM:108:ARG:NH2  | 2.38                     | 0.54              |
| 1:AA:1368:G:H2'    | 1:AA:1369:C:C5'    | 2.33                     | 0.54              |
| 1:AA:477:A:O2'     | 1:AA:479:C:H5'     | 2.07                     | 0.54              |
| 1:AA:563:A:H5'     | 1:AA:566:G:H21     | 1.70                     | 0.54              |
| 1:AA:591:U:C2      | 1:AA:592:G:C8      | 2.95                     | 0.54              |
| 1:AA:609:A:C2'     | 1:AA:610:G:H5'     | 2.37                     | 0.54              |
| 1:AA:848:C:O2'     | 1:AA:849:C:H5'     | 2.08                     | 0.54              |
| 5:AE:64:ARG:HH11   | 5:AE:64:ARG:HG3    | 1.73                     | 0.54              |
| 7:AG:79:ARG:HD3    | 7:AG:79:ARG:N      | 2.23                     | 0.54              |
| 8:AH:123:GLU:O     | 8:AH:127:LEU:HB2   | 2.07                     | 0.54              |
| 12:AL:58:VAL:O     | 12:AL:65:GLU:HA    | 2.08                     | 0.54              |
| 18:AR:84:LYS:N     | 18:AR:84:LYS:HD3   | 2.22                     | 0.54              |
| 22:AV:1:G:C2       | 22:AV:73:A:C8      | 2.95                     | 0.54              |
| 24:AY:498:ILE:HG22 | 24:AY:507:TYR:CD2  | 2.42                     | 0.54              |
| 24:AY:513:LYS:HB2  | 24:AY:566:THR:HB   | 1.89                     | 0.54              |
| 24:AY:89:ASP:O     | 24:AY:90:PHE:CD1   | 2.61                     | 0.54              |
| 35:BA:1652:A:O5'   | 35:BA:1652:A:H8    | 1.91                     | 0.54              |
| 35:BA:2339:G:H2'   | 35:BA:2340:G:C8    | 2.43                     | 0.54              |
| 35:BA:688:U:O2'    | 35:BA:689:A:H5'    | 2.08                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BC:54:ARG:CZ   | 37:BC:56:ASP:HB3   | 2.37                     | 0.54              |
| 37:BC:73:VAL:HG21 | 37:BC:157:ILE:HG22 | 1.88                     | 0.54              |
| 39:BE:179:GLU:CB  | 39:BE:181:LEU:HD23 | 2.28                     | 0.54              |
| 48:BP:108:LYS:O   | 48:BP:110:TYR:N    | 2.41                     | 0.54              |
| 48:BP:17:LYS:O    | 48:BP:17:LYS:HG2   | 2.08                     | 0.54              |
| 48:BP:16:ARG:NH2  | 48:BP:18:ARG:HG2   | 2.22                     | 0.54              |
| 49:BQ:1:MET:HE3   | 49:BQ:1:MET:HA     | 1.90                     | 0.54              |
| 52:BT:35:LYS:NZ   | 52:BT:41:ARG:HD2   | 2.23                     | 0.54              |
| 49:BQ:60:ARG:HA   | 58:BZ:179:ASP:HA   | 1.90                     | 0.54              |
| 1:AA:1077:G:C2    | 1:AA:1081:G:C6     | 2.96                     | 0.54              |
| 1:AA:355:C:H2'    | 1:AA:356:A:O4'     | 2.08                     | 0.54              |
| 1:AA:507:C:H3'    | 1:AA:508:C:H2'     | 1.88                     | 0.54              |
| 1:AA:78:G:H1'     | 1:AA:79:G:O5'      | 2.08                     | 0.54              |
| 2:AB:39:ILE:O     | 2:AB:40:HIS:C      | 2.46                     | 0.54              |
| 3:AC:14:ILE:HG12  | 3:AC:15:THR:N      | 2.17                     | 0.54              |
| 4:AD:129:ASN:HD21 | 4:AD:145:GLU:H     | 1.53                     | 0.54              |
| 11:AK:93:GLN:HA   | 11:AK:93:GLN:OE1   | 2.06                     | 0.54              |
| 16:AP:20:VAL:CG2  | 16:AP:32:TYR:HB2   | 2.38                     | 0.54              |
| 20:AT:27:LYS:HD3  | 20:AT:27:LYS:C     | 2.29                     | 0.54              |
| 22:AV:39:U:O2'    | 22:AV:40:C:H5'     | 2.07                     | 0.54              |
| 24:AY:26:THR:HA   | 24:AY:83:ASP:OD2   | 2.07                     | 0.54              |
| 24:AY:25:LYS:HZ1  | 24:AY:86:GLY:H     | 1.54                     | 0.54              |
| 25:B0:69:PHE:CD1  | 25:B0:69:PHE:N     | 2.75                     | 0.54              |
| 27:B2:21:LEU:O    | 27:B2:24:LEU:N     | 2.41                     | 0.54              |
| 31:B6:15:GLU:CD   | 31:B6:18:ARG:NH1   | 2.62                     | 0.54              |
| 33:B8:62:LEU:C    | 33:B8:64:TYR:H     | 2.11                     | 0.54              |
| 35:BA:1084:A:N7   | 35:BA:1085:A:C5    | 2.76                     | 0.54              |
| 35:BA:1842:G:H2'  | 35:BA:1843:C:C6    | 2.43                     | 0.54              |
| 35:BA:207:A:H2'   | 35:BA:208:C:O4'    | 2.08                     | 0.54              |
| 35:BA:2556:C:H2'  | 35:BA:2557:G:O5'   | 2.08                     | 0.54              |
| 35:BA:259:G:H1'   | 35:BA:621:A:O2'    | 2.07                     | 0.54              |
| 40:BF:34:TRP:HB2  | 48:BP:10:PRO:HB2   | 1.89                     | 0.54              |
| 40:BF:7:TYR:HB3   | 40:BF:16:GLY:H     | 1.73                     | 0.54              |
| 41:BG:91:ARG:HG2  | 41:BG:92:VAL:N     | 2.23                     | 0.54              |
| 47:BO:10:VAL:HG23 | 47:BO:10:VAL:O     | 2.08                     | 0.54              |
| 52:BT:46:GLU:O    | 52:BT:65:LYS:HE3   | 2.07                     | 0.54              |
| 1:AA:1029:C:C4    | 1:AA:1030(A):G:O6  | 2.61                     | 0.54              |
| 1:AA:536:C:H2'    | 1:AA:537:G:H8      | 1.71                     | 0.54              |
| 1:AA:625:G:H2'    | 1:AA:626:U:C6      | 2.42                     | 0.54              |
| 1:AA:679:C:H2'    | 1:AA:680:C:H6      | 1.73                     | 0.54              |
| 1:AA:699:C:C2'    | 1:AA:700:G:C5'     | 2.75                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:83:SER:HA     | 4:AD:89:THR:HG21   | 1.89                     | 0.54              |
| 7:AG:49:ILE:HG22   | 7:AG:53:LYS:HE3    | 1.89                     | 0.54              |
| 19:AS:6:LYS:HG3    | 19:AS:7:LYS:N      | 2.20                     | 0.54              |
| 22:AV:27:G:H1      | 22:AV:43:C:N4      | 2.03                     | 0.54              |
| 24:AY:516:PRO:C    | 24:AY:517:LEU:HD12 | 2.28                     | 0.54              |
| 29:B4:28:LYS:HZ2   | 41:BG:145:THR:H    | 1.56                     | 0.54              |
| 29:B4:6:HIS:CE1    | 41:BG:66:GLN:HG3   | 2.44                     | 0.54              |
| 30:B5:48:GLU:N     | 30:B5:48:GLU:OE1   | 2.39                     | 0.54              |
| 35:BA:1120:G:H2'   | 35:BA:1121:C:C6    | 2.43                     | 0.54              |
| 35:BA:15:G:H2'     | 35:BA:16:G:C5'     | 2.32                     | 0.54              |
| 35:BA:2126:A:N6    | 35:BA:2163:C:H4'   | 2.22                     | 0.54              |
| 35:BA:262:A:C2'    | 35:BA:263:C:C5'    | 2.83                     | 0.54              |
| 35:BA:327:G:H2'    | 35:BA:328:U:O5'    | 2.08                     | 0.54              |
| 35:BA:877:U:O2'    | 35:BA:878:A:H5''   | 2.07                     | 0.54              |
| 39:BE:141:ILE:CB   | 39:BE:154:LYS:HE2  | 2.38                     | 0.54              |
| 39:BE:101:ARG:HB3  | 39:BE:169:ASN:HD22 | 1.72                     | 0.54              |
| 40:BF:126:VAL:HG21 | 40:BF:129:PHE:CZ   | 2.43                     | 0.54              |
| 41:BG:42:GLY:C     | 41:BG:47:LYS:HZ2   | 2.11                     | 0.54              |
| 41:BG:37:VAL:O     | 41:BG:93:THR:O     | 2.25                     | 0.54              |
| 48:BP:9:ASN:H      | 48:BP:10:PRO:HD2   | 1.71                     | 0.54              |
| 51:BS:13:ARG:HG3   | 51:BS:14:VAL:N     | 2.15                     | 0.54              |
| 54:BV:62:LEU:HD21  | 54:BV:95:LEU:CB    | 2.25                     | 0.54              |
| 35:BA:896:A:O4'    | 58:BZ:176:PRO:HG3  | 2.07                     | 0.54              |
| 58:BZ:180:VAL:O    | 58:BZ:181:GLU:HB2  | 2.08                     | 0.54              |
| 1:AA:41:G:H2'      | 1:AA:42:G:C8       | 2.43                     | 0.53              |
| 1:AA:588:G:O6      | 1:AA:753:A:H2'     | 2.08                     | 0.53              |
| 1:AA:699:C:H6      | 1:AA:699:C:O5'     | 1.91                     | 0.53              |
| 1:AA:92:C:C2'      | 1:AA:93:G:H5'      | 2.37                     | 0.53              |
| 3:AC:187:ALA:O     | 3:AC:188:LEU:CB    | 2.55                     | 0.53              |
| 3:AC:35:GLU:HG2    | 3:AC:39:ILE:HD11   | 1.90                     | 0.53              |
| 3:AC:60:ALA:HB3    | 3:AC:63:ASN:HD22   | 1.72                     | 0.53              |
| 5:AE:12:LEU:C      | 5:AE:13:ILE:HD12   | 2.28                     | 0.53              |
| 16:AP:18:ARG:HG3   | 16:AP:35:LYS:HE3   | 1.89                     | 0.53              |
| 24:AY:9:LEU:CD2    | 24:AY:284:LEU:HD13 | 2.38                     | 0.53              |
| 24:AY:25:LYS:NZ    | 24:AY:86:GLY:H     | 2.05                     | 0.53              |
| 35:BA:1231:G:H2'   | 35:BA:1232:G:C8    | 2.43                     | 0.53              |
| 35:BA:1301:A:N3    | 35:BA:1301:A:C5'   | 2.71                     | 0.53              |
| 35:BA:1446:C:H41   | 35:BA:1465:G:H1    | 1.49                     | 0.53              |
| 35:BA:18:C:O2      | 35:BA:19:C:C5      | 2.60                     | 0.53              |
| 35:BA:2000:G:N3    | 35:BA:2001:A:C8    | 2.75                     | 0.53              |
| 35:BA:2328:A:H2'   | 35:BA:2329:G:C8    | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BA:250:G:C6    | 35:BA:251:A:C6    | 2.96                     | 0.53              |
| 39:BE:111:ARG:HB3 | 50:BR:2:ARG:CZ    | 2.39                     | 0.53              |
| 39:BE:87:GLU:OE1  | 39:BE:89:ASP:HB3  | 2.08                     | 0.53              |
| 40:BF:27:GLU:OE1  | 40:BF:27:GLU:N    | 2.41                     | 0.53              |
| 41:BG:113:ARG:HG2 | 41:BG:141:PHE:CD2 | 2.43                     | 0.53              |
| 41:BG:60:LEU:HD12 | 41:BG:60:LEU:O    | 2.08                     | 0.53              |
| 48:BP:24:GLY:HA3  | 48:BP:29:LYS:O    | 2.08                     | 0.53              |
| 48:BP:66:GLY:O    | 48:BP:67:MET:CB   | 2.56                     | 0.53              |
| 51:BS:39:ILE:O    | 51:BS:39:ILE:HG22 | 2.08                     | 0.53              |
| 52:BT:91:ARG:O    | 52:BT:117:ASP:HB2 | 2.07                     | 0.53              |
| 53:BU:17:ILE:HG23 | 53:BU:39:LEU:HD12 | 1.89                     | 0.53              |
| 53:BU:90:VAL:O    | 53:BU:91:ASP:C    | 2.47                     | 0.53              |
| 1:AA:1047:G:H2'   | 1:AA:1048:G:C5'   | 2.24                     | 0.53              |
| 1:AA:1372:U:H2'   | 1:AA:1373:G:O5'   | 2.07                     | 0.53              |
| 1:AA:188:C:O2'    | 1:AA:189:G:H5'    | 2.08                     | 0.53              |
| 2:AB:169:LYS:O    | 2:AB:169:LYS:HD3  | 2.08                     | 0.53              |
| 3:AC:35:GLU:OE1   | 3:AC:97:LYS:HE2   | 2.08                     | 0.53              |
| 7:AG:113:GLU:HB2  | 7:AG:119:ARG:HD2  | 1.90                     | 0.53              |
| 7:AG:38:LEU:O     | 7:AG:42:ILE:HG13  | 2.08                     | 0.53              |
| 7:AG:48:LYS:HG2   | 7:AG:49:ILE:N     | 2.22                     | 0.53              |
| 9:AI:121:ARG:NH1  | 9:AI:121:ARG:HG2  | 2.22                     | 0.53              |
| 7:AG:16:LEU:CD1   | 9:AI:42:ARG:HA    | 2.39                     | 0.53              |
| 24:AY:617:MET:CE  | 24:AY:641:GLN:HG2 | 2.38                     | 0.53              |
| 25:B0:76:GLY:O    | 25:B0:78:TYR:CE1  | 2.60                     | 0.53              |
| 26:B1:49:VAL:HG13 | 26:B1:60:PHE:HB2  | 1.91                     | 0.53              |
| 27:B2:70:GLN:HE21 | 27:B2:71:ASN:HB2  | 1.73                     | 0.53              |
| 31:B6:53:LYS:O    | 31:B6:54:ILE:OXT  | 2.25                     | 0.53              |
| 35:BA:1063:G:H22  | 35:BA:1074:G:H1   | 1.56                     | 0.53              |
| 35:BA:1475:G:C8   | 35:BA:1475:G:H5'  | 2.37                     | 0.53              |
| 35:BA:1587:A:H3'  | 35:BA:1588:C:C6   | 2.43                     | 0.53              |
| 35:BA:2753:A:C2'  | 35:BA:2754:U:C5'  | 2.85                     | 0.53              |
| 35:BA:955:C:OP2   | 49:BQ:14:ARG:CD   | 2.55                     | 0.53              |
| 36:BB:30:C:H1'    | 36:BB:57:A:H61    | 1.72                     | 0.53              |
| 53:BU:15:LYS:O    | 53:BU:19:LYS:HD3  | 2.08                     | 0.53              |
| 57:BY:26:LYS:CG   | 57:BY:27:VAL:H    | 2.18                     | 0.53              |
| 1:AA:1241:G:H2'   | 1:AA:1242:C:H6    | 1.69                     | 0.53              |
| 1:AA:1305:G:H1'   | 1:AA:1332:A:H62   | 1.73                     | 0.53              |
| 1:AA:152:A:H62    | 1:AA:169:C:H42    | 1.57                     | 0.53              |
| 1:AA:263:A:OP2    | 20:AT:79:ARG:NH1  | 2.40                     | 0.53              |
| 1:AA:36:C:O2'     | 1:AA:37:U:H5'     | 2.08                     | 0.53              |
| 1:AA:64:G:C4'     | 1:AA:65:U:OP1     | 2.56                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AK:48:ILE:HD11  | 11:AK:64:ALA:HA    | 1.90                     | 0.53              |
| 12:AL:75:HIS:CD2   | 12:AL:77:LEU:H     | 2.23                     | 0.53              |
| 17:AQ:40:LYS:HD3   | 17:AQ:42:TYR:CZ    | 2.43                     | 0.53              |
| 24:AY:58:GLU:HG2   | 24:AY:63:ILE:O     | 2.08                     | 0.53              |
| 25:B0:10:THR:CG2   | 25:B0:11:ARG:H     | 2.02                     | 0.53              |
| 25:B0:69:PHE:CD2   | 25:B0:79:VAL:HG22  | 2.43                     | 0.53              |
| 27:B2:11:GLU:O     | 27:B2:15:LYS:HG2   | 2.09                     | 0.53              |
| 29:B4:71:ARG:O     | 29:B4:71:ARG:HG3   | 2.08                     | 0.53              |
| 35:BA:1516:C:C2'   | 35:BA:1517:G:H5''  | 2.37                     | 0.53              |
| 35:BA:177:G:N3     | 35:BA:177:G:H2'    | 2.23                     | 0.53              |
| 35:BA:265:A:H1'    | 35:BA:266:G:O4'    | 2.08                     | 0.53              |
| 35:BA:2838:G:O2'   | 50:BR:45:ARG:HD3   | 2.08                     | 0.53              |
| 35:BA:686:G:N2     | 35:BA:788:A:H61    | 2.06                     | 0.53              |
| 37:BC:103:LYS:HZ2  | 37:BC:103:LYS:HB2  | 1.74                     | 0.53              |
| 37:BC:106:ASP:O    | 37:BC:107:GLY:C    | 2.46                     | 0.53              |
| 37:BC:127:LYS:H    | 37:BC:127:LYS:HD3  | 1.73                     | 0.53              |
| 40:BF:140:LEU:O    | 40:BF:143:ALA:HB3  | 2.07                     | 0.53              |
| 41:BG:104:GLU:C    | 41:BG:106:LEU:H    | 2.12                     | 0.53              |
| 41:BG:77:ILE:CG2   | 41:BG:80:PHE:HB2   | 2.32                     | 0.53              |
| 41:BG:9:ARG:HD2    | 41:BG:9:ARG:N      | 2.23                     | 0.53              |
| 42:BH:124:GLU:HB2  | 42:BH:132:ARG:HG2  | 1.90                     | 0.53              |
| 47:BO:34:THR:HG22  | 47:BO:37:ASP:OD2   | 2.08                     | 0.53              |
| 50:BR:13:HIS:CE1   | 50:BR:16:HIS:HB2   | 2.43                     | 0.53              |
| 53:BU:24:TYR:HB2   | 53:BU:29:SER:HB3   | 1.89                     | 0.53              |
| 1:AA:266:G:O2'     | 1:AA:267:C:H5''    | 2.08                     | 0.53              |
| 1:AA:359:U:C2'     | 1:AA:360:A:C5'     | 2.87                     | 0.53              |
| 1:AA:937:A:H2'     | 1:AA:938:A:H5'     | 1.90                     | 0.53              |
| 2:AB:39:ILE:O      | 2:AB:41:ILE:CD1    | 2.57                     | 0.53              |
| 8:AH:72:PRO:O      | 8:AH:73:ASP:HB3    | 2.08                     | 0.53              |
| 10:AJ:90:LEU:O     | 10:AJ:90:LEU:HG    | 2.08                     | 0.53              |
| 24:AY:402:ILE:HG22 | 24:AY:403:GLU:N    | 2.23                     | 0.53              |
| 24:AY:69:VAL:O     | 24:AY:69:VAL:HG13  | 2.08                     | 0.53              |
| 25:B0:53:MET:HE1   | 25:B0:57:PHE:CD2   | 2.43                     | 0.53              |
| 35:BA:1427:A:C4'   | 35:BA:1428:C:O5'   | 2.40                     | 0.53              |
| 35:BA:1451:C:H2'   | 35:BA:1458:C:H41   | 1.73                     | 0.53              |
| 35:BA:1528:A:N1    | 35:BA:1542:A:H2    | 2.07                     | 0.53              |
| 35:BA:2310:A:N7    | 41:BG:75:LYS:HE2   | 2.24                     | 0.53              |
| 35:BA:2712:U:H1'   | 35:BA:2712(A):A:N7 | 2.23                     | 0.53              |
| 35:BA:2717:G:O2'   | 52:BT:96:ARG:HD3   | 2.09                     | 0.53              |
| 35:BA:419:C:H2'    | 35:BA:420:C:H6     | 1.72                     | 0.53              |
| 35:BA:843:G:O2'    | 35:BA:844:C:H5'    | 2.09                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:860:U:H5'    | 35:BA:860:U:O2    | 2.08                     | 0.53              |
| 37:BC:100:ILE:O    | 37:BC:102:GLN:N   | 2.42                     | 0.53              |
| 41:BG:131:TYR:O    | 41:BG:132:ASN:CB  | 2.55                     | 0.53              |
| 41:BG:94:LEU:N     | 41:BG:94:LEU:HD22 | 2.22                     | 0.53              |
| 44:BK:56:UNK:C     | 44:BK:67:UNK:HA   | 2.38                     | 0.53              |
| 50:BR:101:ALA:O    | 50:BR:102:GLU:HB2 | 2.08                     | 0.53              |
| 51:BS:88:ASP:CG    | 51:BS:89:ARG:N    | 2.61                     | 0.53              |
| 55:BW:1:MET:HB3    | 55:BW:64:MET:CE   | 2.38                     | 0.53              |
| 1:AA:1279:A:H2'    | 1:AA:1282:C:N4    | 2.24                     | 0.53              |
| 1:AA:1347:G:N7     | 9:AI:10:ARG:NH2   | 2.56                     | 0.53              |
| 1:AA:1504:G:P      | 1:AA:1504:G:H3'   | 2.48                     | 0.53              |
| 1:AA:199:G:C2'     | 1:AA:200:G:O5'    | 2.57                     | 0.53              |
| 1:AA:701:C:OP1     | 1:AA:703:G:H5'    | 2.09                     | 0.53              |
| 2:AB:15:VAL:HG13   | 2:AB:209:ARG:HB3  | 1.91                     | 0.53              |
| 2:AB:89:GLY:O      | 2:AB:90:MET:CG    | 2.30                     | 0.53              |
| 4:AD:170:VAL:HG21  | 4:AD:176:LEU:HB2  | 1.90                     | 0.53              |
| 7:AG:46:ALA:HB1    | 7:AG:121:ALA:HB2  | 1.89                     | 0.53              |
| 9:AI:11:LYS:HG3    | 9:AI:11:LYS:O     | 2.09                     | 0.53              |
| 10:AJ:89:ASP:O     | 10:AJ:90:LEU:HB2  | 2.09                     | 0.53              |
| 13:AM:65:LYS:O     | 13:AM:65:LYS:HG3  | 2.08                     | 0.53              |
| 24:AY:342:TYR:CZ   | 24:AY:347:GLY:HA2 | 2.44                     | 0.53              |
| 24:AY:408:VAL:HG12 | 24:AY:656:ALA:HB2 | 1.89                     | 0.53              |
| 24:AY:689:LYS:HG3  | 24:AY:690:GLY:N   | 2.23                     | 0.53              |
| 29:B4:32:TYR:CD2   | 29:B4:33:VAL:O    | 2.62                     | 0.53              |
| 35:BA:1122:G:C2    | 35:BA:1123:C:C5   | 2.97                     | 0.53              |
| 35:BA:1145:C:O2'   | 35:BA:1146:C:H5'  | 2.09                     | 0.53              |
| 35:BA:1300:U:H1'   | 35:BA:1301:A:OP2  | 2.09                     | 0.53              |
| 35:BA:1413:G:C2'   | 35:BA:1414:G:O5'  | 2.56                     | 0.53              |
| 35:BA:1539:G:C6    | 35:BA:1540:U:H1'  | 2.43                     | 0.53              |
| 35:BA:1798:U:H5    | 38:BD:274:ARG:NH2 | 2.06                     | 0.53              |
| 35:BA:2022:U:O2'   | 35:BA:2617:C:H5'  | 2.07                     | 0.53              |
| 35:BA:2312:U:H2'   | 35:BA:2313:C:C5'  | 2.10                     | 0.53              |
| 35:BA:2373:G:H2'   | 35:BA:2374:C:C6   | 2.44                     | 0.53              |
| 35:BA:244:A:C2     | 35:BA:255:A:C4    | 2.97                     | 0.53              |
| 35:BA:2779:U:H1'   | 35:BA:2781:A:C6   | 2.44                     | 0.53              |
| 35:BA:492:A:C2'    | 35:BA:493:G:H5'   | 2.39                     | 0.53              |
| 35:BA:755:C:H2'    | 35:BA:756:C:H6    | 1.74                     | 0.53              |
| 35:BA:900:A:H3'    | 35:BA:901:A:C8    | 2.41                     | 0.53              |
| 37:BC:124:VAL:CG1  | 37:BC:125:GLY:N   | 2.71                     | 0.53              |
| 38:BD:134:ARG:CZ   | 38:BD:135:PHE:HE1 | 2.20                     | 0.53              |
| 41:BG:53:LEU:C     | 41:BG:55:LYS:H    | 2.11                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:2467:C:H4'   | 49:BQ:123:HIS:CD2 | 2.43                     | 0.53              |
| 55:BW:20:VAL:HG23  | 55:BW:47:VAL:HG21 | 1.90                     | 0.53              |
| 1:AA:105:G:C6      | 1:AA:106:C:N3     | 2.77                     | 0.53              |
| 1:AA:436:C:H2'     | 1:AA:437:U:H6     | 1.72                     | 0.53              |
| 1:AA:592:G:C2'     | 1:AA:593:G:H5'    | 2.38                     | 0.53              |
| 1:AA:942:G:C2      | 1:AA:943:U:C2     | 2.97                     | 0.53              |
| 2:AB:74:LYS:O      | 2:AB:75:LYS:C     | 2.46                     | 0.53              |
| 13:AM:23:TYR:HB3   | 13:AM:67:GLU:HA   | 1.91                     | 0.53              |
| 20:AT:64:ASP:OD1   | 20:AT:81:LYS:HD2  | 2.07                     | 0.53              |
| 24:AY:312:LEU:HD23 | 24:AY:387:ASP:O   | 2.08                     | 0.53              |
| 24:AY:5:VAL:HG13   | 24:AY:6:GLU:H     | 1.74                     | 0.53              |
| 25:B0:35:ASN:O     | 25:B0:37:LEU:HD22 | 2.08                     | 0.53              |
| 25:B0:21:LEU:HD13  | 25:B0:41:ARG:HG2  | 1.90                     | 0.53              |
| 27:B2:69:ARG:O     | 27:B2:70:GLN:CD   | 2.47                     | 0.53              |
| 31:B6:15:GLU:OE2   | 31:B6:41:PRO:CB   | 2.56                     | 0.53              |
| 31:B6:17:LYS:HB2   | 31:B6:18:ARG:NH1  | 2.19                     | 0.53              |
| 35:BA:1050:A:H2'   | 35:BA:1051:G:H8   | 1.74                     | 0.53              |
| 35:BA:11:G:O5'     | 35:BA:11:G:H8     | 1.90                     | 0.53              |
| 35:BA:1227:G:C4    | 35:BA:1228:G:C8   | 2.96                     | 0.53              |
| 35:BA:1291:C:HO2'  | 35:BA:1292:U:H5'  | 1.70                     | 0.53              |
| 35:BA:1461:G:C6    | 35:BA:1462:C:N4   | 2.76                     | 0.53              |
| 35:BA:14:A:H8      | 35:BA:14:A:O5'    | 1.91                     | 0.53              |
| 35:BA:1684:C:O2'   | 35:BA:1685:C:H5'  | 2.09                     | 0.53              |
| 35:BA:1767:C:H2'   | 35:BA:1768:U:C5'  | 2.29                     | 0.53              |
| 35:BA:2092:U:H5    | 35:BA:2226:C:OP2  | 1.91                     | 0.53              |
| 35:BA:2363:C:O2'   | 35:BA:2364:C:C5'  | 2.39                     | 0.53              |
| 35:BA:2363:C:H2'   | 35:BA:2364:C:H6   | 1.72                     | 0.53              |
| 35:BA:2403:C:P     | 35:BA:2403:C:C6   | 3.01                     | 0.53              |
| 35:BA:2491:U:H4'   | 35:BA:2570:G:OP1  | 2.09                     | 0.53              |
| 35:BA:2758:A:C4    | 35:BA:2759:G:C8   | 2.97                     | 0.53              |
| 35:BA:632:A:H8     | 35:BA:632:A:O5'   | 1.90                     | 0.53              |
| 35:BA:813:U:O2'    | 35:BA:1225:G:H1'  | 2.09                     | 0.53              |
| 37:BC:128:LEU:HD12 | 37:BC:128:LEU:O   | 2.09                     | 0.53              |
| 38:BD:92:ILE:HA    | 38:BD:107:ALA:H   | 1.74                     | 0.53              |
| 39:BE:101:ARG:HB3  | 39:BE:169:ASN:ND2 | 2.24                     | 0.53              |
| 35:BA:672:C:O3'    | 40:BF:81:PRO:HG2  | 2.08                     | 0.53              |
| 41:BG:39:ILE:HD11  | 41:BG:155:MET:SD  | 2.48                     | 0.53              |
| 51:BS:19:LYS:O     | 51:BS:19:LYS:HG2  | 2.09                     | 0.53              |
| 54:BV:47:VAL:O     | 54:BV:49:THR:N    | 2.41                     | 0.53              |
| 55:BW:13:SER:HB3   | 55:BW:16:LYS:HD2  | 1.89                     | 0.53              |
| 55:BW:26:GLY:N     | 55:BW:71:VAL:HG23 | 2.21                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:696:A:O5'    | 1:AA:696:A:H8     | 1.91                     | 0.53              |
| 1:AA:92:C:H2'     | 1:AA:93:G:C5'     | 2.38                     | 0.53              |
| 4:AD:170:VAL:HG12 | 4:AD:174:LEU:HB2  | 1.91                     | 0.53              |
| 4:AD:34:GLU:O     | 4:AD:35:ARG:HB2   | 2.08                     | 0.53              |
| 1:AA:1372:U:OP2   | 9:AI:11:LYS:HE3   | 2.07                     | 0.53              |
| 10:AJ:8:LEU:HD12  | 10:AJ:8:LEU:H     | 1.73                     | 0.53              |
| 12:AL:27:LEU:HD12 | 12:AL:28:LYS:CE   | 2.28                     | 0.53              |
| 19:AS:7:LYS:O     | 19:AS:7:LYS:CG    | 2.56                     | 0.53              |
| 24:AY:99:ARG:NH1  | 24:AY:402:ILE:C   | 2.62                     | 0.53              |
| 25:B0:4:LYS:O     | 25:B0:5:LYS:C     | 2.47                     | 0.53              |
| 26:B1:57:GLU:O    | 26:B1:58:ILE:CG1  | 2.54                     | 0.53              |
| 29:B4:12:ALA:O    | 29:B4:13:ARG:HG2  | 2.09                     | 0.53              |
| 31:B6:20:ASN:CG   | 31:B6:21:TYR:H    | 2.12                     | 0.53              |
| 35:BA:1021:A:O2'  | 35:BA:1023:U:H5'' | 2.08                     | 0.53              |
| 35:BA:1839:G:C8   | 35:BA:1839:G:H5'  | 2.42                     | 0.53              |
| 35:BA:2000:G:N2   | 35:BA:2001:A:C8   | 2.75                     | 0.53              |
| 35:BA:2262:U:O2'  | 35:BA:2263:C:H5'  | 2.09                     | 0.53              |
| 35:BA:597:U:O2'   | 48:BP:15:ARG:HG2  | 2.08                     | 0.53              |
| 35:BA:888:C:O2'   | 35:BA:889:C:H5''  | 2.08                     | 0.53              |
| 35:BA:963:U:C2'   | 35:BA:964:C:O5'   | 2.56                     | 0.53              |
| 37:BC:65:LEU:HD22 | 37:BC:189:ASN:HB3 | 1.91                     | 0.53              |
| 47:BO:98:VAL:HG12 | 47:BO:117:LEU:HB3 | 1.89                     | 0.53              |
| 51:BS:68:GLN:C    | 51:BS:70:GLY:N    | 2.62                     | 0.53              |
| 51:BS:88:ASP:OD1  | 51:BS:89:ARG:N    | 2.42                     | 0.53              |
| 54:BV:47:VAL:HB   | 54:BV:49:THR:O    | 2.09                     | 0.53              |
| 57:BY:57:GLN:HA   | 57:BY:57:GLN:OE1  | 2.08                     | 0.53              |
| 1:AA:1048:G:N3    | 1:AA:1050:G:C8    | 2.77                     | 0.53              |
| 1:AA:1298:C:H4'   | 1:AA:1299:A:C4    | 2.44                     | 0.53              |
| 1:AA:1370:G:H2'   | 1:AA:1371:G:H5'   | 1.91                     | 0.53              |
| 1:AA:198:G:O2'    | 1:AA:199:G:P      | 2.66                     | 0.53              |
| 1:AA:543:C:O2'    | 1:AA:544:G:H5''   | 2.09                     | 0.53              |
| 1:AA:609:A:H2'    | 1:AA:610:G:H5'    | 1.91                     | 0.53              |
| 1:AA:790:A:H5'    | 22:AV:38:A:O3'    | 2.09                     | 0.53              |
| 1:AA:89:C:O2'     | 1:AA:90:U:H6      | 1.92                     | 0.53              |
| 3:AC:12:LEU:O     | 3:AC:13:GLY:C     | 2.47                     | 0.53              |
| 6:AF:45:LEU:O     | 6:AF:46:ARG:HG2   | 2.08                     | 0.53              |
| 12:AL:46:LYS:O    | 12:AL:48:PRO:CD   | 2.57                     | 0.53              |
| 16:AP:10:GLY:CA   | 16:AP:16:HIS:HB2  | 2.39                     | 0.53              |
| 24:AY:229:LEU:C   | 24:AY:231:TYR:H   | 2.12                     | 0.53              |
| 27:B2:21:LEU:HD13 | 27:B2:64:LEU:HB2  | 1.90                     | 0.53              |
| 27:B2:41:ILE:HD12 | 27:B2:43:GLN:CG   | 2.34                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:B2:31:GLU:HB3   | 27:B2:53:LEU:HD11  | 1.91                     | 0.53              |
| 32:B7:8:ASN:C      | 32:B7:8:ASN:ND2    | 2.52                     | 0.53              |
| 35:BA:1252:G:OP2   | 53:BU:14:HIS:HE1   | 1.91                     | 0.53              |
| 35:BA:1771:C:C1'   | 35:BA:1786:A:H8    | 2.22                     | 0.53              |
| 35:BA:2150:U:H2'   | 35:BA:2151:G:C8    | 2.43                     | 0.53              |
| 35:BA:2404:C:H2'   | 35:BA:2405:G:O5'   | 2.09                     | 0.53              |
| 35:BA:2801:A:O2'   | 35:BA:2895:U:H5'   | 2.08                     | 0.53              |
| 37:BC:116:ALA:HB1  | 37:BC:118:PRO:HA   | 1.91                     | 0.53              |
| 38:BD:206:LEU:HD23 | 38:BD:211:ARG:NH1  | 2.24                     | 0.53              |
| 40:BF:46:ARG:HG3   | 40:BF:46:ARG:HH11  | 1.74                     | 0.53              |
| 35:BA:1258:C:O4'   | 40:BF:84:VAL:HG11  | 2.08                     | 0.53              |
| 42:BH:166:GLY:O    | 42:BH:167:GLU:HB2  | 2.09                     | 0.53              |
| 46:BN:46:VAL:HG13  | 46:BN:48:MET:HG2   | 1.90                     | 0.53              |
| 50:BR:21:TYR:OH    | 50:BR:43:GLU:HG2   | 2.09                     | 0.53              |
| 50:BR:70:LEU:HD13  | 50:BR:75:LEU:CD1   | 2.39                     | 0.53              |
| 52:BT:93:ARG:CG    | 52:BT:117:ASP:HA   | 2.36                     | 0.53              |
| 58:BZ:40:ASP:OD1   | 58:BZ:42:VAL:HG12  | 2.09                     | 0.53              |
| 7:AG:47:CYS:HA     | 7:AG:50:ILE:CG2    | 2.39                     | 0.53              |
| 10:AJ:4:ILE:HG21   | 10:AJ:74:ILE:HD11  | 1.91                     | 0.53              |
| 10:AJ:37:PRO:HA    | 10:AJ:72:VAL:HG22  | 1.91                     | 0.53              |
| 16:AP:3:LYS:O      | 16:AP:21:VAL:HA    | 2.09                     | 0.53              |
| 19:AS:40:ILE:HG23  | 19:AS:67:VAL:HA    | 1.91                     | 0.53              |
| 31:B6:16:CYS:SG    | 31:B6:48:VAL:HG23  | 2.48                     | 0.53              |
| 35:BA:1821:A:O5'   | 35:BA:1821:A:H8    | 1.92                     | 0.53              |
| 35:BA:1984:G:H2'   | 35:BA:1985:G:C5'   | 2.37                     | 0.53              |
| 35:BA:2317:C:H2'   | 35:BA:2318:G:H5'   | 1.91                     | 0.53              |
| 37:BC:108:TRP:C    | 37:BC:110:ASP:N    | 2.62                     | 0.53              |
| 37:BC:116:ALA:CB   | 37:BC:118:PRO:HA   | 2.37                     | 0.53              |
| 39:BE:93:VAL:HG12  | 39:BE:182:LEU:HD13 | 1.91                     | 0.53              |
| 35:BA:558:G:OP1    | 46:BN:111:PRO:HD2  | 2.09                     | 0.53              |
| 46:BN:119:ARG:HH11 | 46:BN:119:ARG:CG   | 2.22                     | 0.53              |
| 46:BN:22:THR:HG22  | 46:BN:61:ARG:HB3   | 1.91                     | 0.53              |
| 49:BQ:65:PHE:CD1   | 49:BQ:65:PHE:N     | 2.77                     | 0.53              |
| 52:BT:106:SER:C    | 52:BT:107:ASP:OD1  | 2.47                     | 0.53              |
| 52:BT:34:VAL:HG13  | 52:BT:39:ARG:HA    | 1.90                     | 0.53              |
| 57:BY:38:ILE:CG2   | 57:BY:39:VAL:N     | 2.72                     | 0.53              |
| 58:BZ:112:ARG:O    | 58:BZ:112:ARG:HD3  | 2.09                     | 0.53              |
| 1:AA:106:C:O2'     | 1:AA:107:G:C5'     | 2.30                     | 0.53              |
| 1:AA:1125:U:O4     | 10:AJ:5:ARG:NE     | 2.41                     | 0.53              |
| 1:AA:770:C:C2'     | 1:AA:771:G:C5'     | 2.86                     | 0.53              |
| 1:AA:868:C:C2'     | 1:AA:869:G:H5'     | 2.39                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:AE:6:PHE:CB      | 5:AE:34:VAL:HG22  | 2.39                     | 0.53              |
| 24:AY:17:ILE:N     | 24:AY:17:ILE:HD12 | 2.24                     | 0.53              |
| 24:AY:459:LEU:HD12 | 24:AY:459:LEU:N   | 2.23                     | 0.53              |
| 35:BA:1104:C:C2'   | 35:BA:1105:U:C5'  | 2.82                     | 0.53              |
| 35:BA:1121:C:H2'   | 35:BA:1122:G:O5'  | 2.09                     | 0.53              |
| 35:BA:1272:A:OP2   | 35:BA:1647:G:OP1  | 2.26                     | 0.53              |
| 35:BA:1301:A:C4'   | 35:BA:1302:A:OP1  | 2.56                     | 0.53              |
| 35:BA:1412:A:HO2'  | 35:BA:1413:G:H5'  | 1.72                     | 0.53              |
| 35:BA:1458:C:H4'   | 35:BA:1459:G:O5'  | 2.09                     | 0.53              |
| 35:BA:1694:C:H4'   | 35:BA:1695:G:H5'' | 1.91                     | 0.53              |
| 35:BA:1711:C:O2'   | 35:BA:1712:C:H5'  | 2.08                     | 0.53              |
| 33:B8:39:LYS:HE3   | 35:BA:2365:G:O6   | 2.09                     | 0.53              |
| 35:BA:2584:U:C2'   | 35:BA:2585:U:H5'  | 2.38                     | 0.53              |
| 35:BA:2649:U:H2'   | 35:BA:2650:U:C6   | 2.44                     | 0.53              |
| 35:BA:402:A:O2'    | 35:BA:403:U:H5'   | 2.09                     | 0.53              |
| 35:BA:523:C:HO2'   | 35:BA:524:U:H5'   | 1.65                     | 0.53              |
| 36:BB:91:C:H5'     | 49:BQ:18:LYS:HG2  | 1.91                     | 0.53              |
| 37:BC:52:PRO:HG2   | 37:BC:53:ARG:H    | 1.73                     | 0.53              |
| 40:BF:50:SER:HB2   | 40:BF:94:PRO:HD3  | 1.90                     | 0.53              |
| 48:BP:101:VAL:CG2  | 48:BP:102:ARG:N   | 2.71                     | 0.53              |
| 53:BU:95:LEU:HD12  | 54:BV:11:GLN:HG3  | 1.91                     | 0.53              |
| 54:BV:39:LEU:HA    | 54:BV:47:VAL:CG1  | 2.38                     | 0.53              |
| 54:BV:49:THR:O     | 54:BV:50:PRO:C    | 2.47                     | 0.53              |
| 53:BU:50:ARG:NH1   | 54:BV:72:VAL:HG12 | 2.19                     | 0.53              |
| 1:AA:1029:C:C3'    | 1:AA:1030:C:C5'   | 2.80                     | 0.52              |
| 1:AA:1400:C:H3'    | 1:AA:1401:G:H5'   | 1.91                     | 0.52              |
| 1:AA:1487:G:H2'    | 1:AA:1488:G:H5'   | 1.90                     | 0.52              |
| 1:AA:46:G:O2'      | 1:AA:365:U:O2'    | 2.25                     | 0.52              |
| 1:AA:406:G:H5''    | 4:AD:5:ILE:CG2    | 2.39                     | 0.52              |
| 1:AA:447:G:H2'     | 1:AA:485:G:N2     | 2.23                     | 0.52              |
| 1:AA:627:G:O2'     | 1:AA:628:G:H5'    | 2.07                     | 0.52              |
| 2:AB:114:ARG:HG3   | 2:AB:114:ARG:NH1  | 2.15                     | 0.52              |
| 13:AM:70:LEU:O     | 13:AM:73:GLU:HB2  | 2.09                     | 0.52              |
| 24:AY:498:ILE:HA   | 24:AY:507:TYR:CB  | 2.39                     | 0.52              |
| 29:B4:16:CYS:HA    | 29:B4:33:VAL:CG1  | 2.39                     | 0.52              |
| 35:BA:1461:G:O2'   | 35:BA:1462:C:H5'  | 2.09                     | 0.52              |
| 35:BA:1494:A:H2'   | 35:BA:1495:A:C5'  | 2.38                     | 0.52              |
| 35:BA:1541:G:H1'   | 35:BA:1542:A:C4   | 2.44                     | 0.52              |
| 35:BA:174:C:O2     | 35:BA:174:C:H2'   | 2.08                     | 0.52              |
| 35:BA:2011:U:H2'   | 35:BA:2012:G:O5'  | 2.09                     | 0.52              |
| 35:BA:2401:U:H5''  | 35:BA:2402:C:C5   | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2611:U:OP2   | 35:BA:2611:U:C6    | 2.61                     | 0.52              |
| 35:BA:375:C:H2'    | 35:BA:376:C:C6     | 2.44                     | 0.52              |
| 37:BC:138:LEU:HD23 | 37:BC:139:PRO:HD2  | 1.90                     | 0.52              |
| 37:BC:88:GLU:HB2   | 37:BC:91:GLY:O     | 2.09                     | 0.52              |
| 38:BD:218:ARG:HH11 | 38:BD:218:ARG:HG3  | 1.74                     | 0.52              |
| 39:BE:116:VAL:HG13 | 39:BE:122:PHE:HB2  | 1.90                     | 0.52              |
| 40:BF:162:LEU:H    | 40:BF:162:LEU:HD12 | 1.74                     | 0.52              |
| 41:BG:135:LEU:O    | 41:BG:137:GLU:N    | 2.31                     | 0.52              |
| 41:BG:154:GLY:O    | 41:BG:155:MET:HB3  | 2.09                     | 0.52              |
| 46:BN:15:LEU:HD12  | 46:BN:136:GLU:CG   | 2.39                     | 0.52              |
| 52:BT:50:ILE:HA    | 52:BT:99:LEU:HD12  | 1.90                     | 0.52              |
| 52:BT:89:VAL:HG12  | 52:BT:91:ARG:H     | 1.74                     | 0.52              |
| 1:AA:1052:U:H6     | 1:AA:1052:U:O5'    | 1.92                     | 0.52              |
| 1:AA:108:G:H5''    | 1:AA:108:G:N3      | 2.23                     | 0.52              |
| 1:AA:1156:G:H8     | 1:AA:1156:G:O5'    | 1.91                     | 0.52              |
| 1:AA:275:G:H5'     | 17:AQ:14:LYS:HD3   | 1.91                     | 0.52              |
| 1:AA:406:G:H1'     | 1:AA:495:A:N1      | 2.24                     | 0.52              |
| 2:AB:54:THR:HG23   | 2:AB:185:ILE:CG2   | 2.40                     | 0.52              |
| 2:AB:36:ARG:O      | 2:AB:37:ASN:HB2    | 2.08                     | 0.52              |
| 3:AC:116:VAL:C     | 3:AC:118:GLN:H     | 2.12                     | 0.52              |
| 7:AG:59:LEU:C      | 7:AG:59:LEU:HD23   | 2.29                     | 0.52              |
| 7:AG:94:ARG:HH11   | 7:AG:94:ARG:HG3    | 1.73                     | 0.52              |
| 8:AH:35:ILE:HG22   | 8:AH:39:LEU:CD2    | 2.38                     | 0.52              |
| 15:AO:23:GLY:O     | 15:AO:24:SER:O     | 2.28                     | 0.52              |
| 16:AP:20:VAL:CG2   | 16:AP:21:VAL:N     | 2.71                     | 0.52              |
| 20:AT:74:LYS:HG3   | 20:AT:75:ASN:ND2   | 2.23                     | 0.52              |
| 24:AY:99:ARG:NE    | 24:AY:128:TYR:CE2  | 2.69                     | 0.52              |
| 24:AY:490:PRO:HB3  | 24:AY:515:GLU:HB3  | 1.91                     | 0.52              |
| 26:B1:30:VAL:O     | 35:BA:2395:C:O2'   | 2.26                     | 0.52              |
| 28:B3:22:ALA:HA    | 28:B3:46:ASN:ND2   | 2.23                     | 0.52              |
| 29:B4:21:VAL:HG11  | 29:B4:35:VAL:HG22  | 1.91                     | 0.52              |
| 29:B4:39:CYS:CB    | 29:B4:41:PRO:CD    | 2.86                     | 0.52              |
| 35:BA:1419:A:O2'   | 35:BA:1420:U:C5'   | 2.54                     | 0.52              |
| 35:BA:1601:G:C5    | 35:BA:1602:U:C4    | 2.98                     | 0.52              |
| 35:BA:1695:G:C3'   | 35:BA:1695:G:N3    | 2.71                     | 0.52              |
| 35:BA:185:U:H4'    | 35:BA:218:A:H4'    | 1.90                     | 0.52              |
| 35:BA:1925:C:C5    | 35:BA:1926:U:H5    | 2.28                     | 0.52              |
| 35:BA:2554:U:O2'   | 35:BA:2555:U:H5'   | 2.09                     | 0.52              |
| 35:BA:331:A:HO2'   | 35:BA:332:A:P      | 2.31                     | 0.52              |
| 37:BC:118:PRO:CB   | 37:BC:121:MET:HG2  | 2.40                     | 0.52              |
| 37:BC:51:ASP:OD2   | 37:BC:54:ARG:HB2   | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BD:16:MET:HB3  | 38:BD:207:GLY:HA3 | 1.91                     | 0.52              |
| 41:BG:111:LEU:HB2 | 41:BG:112:PRO:HD3 | 1.92                     | 0.52              |
| 42:BH:83:TYR:HB3  | 42:BH:134:SER:CA  | 2.36                     | 0.52              |
| 46:BN:35:ARG:NH2  | 46:BN:42:TRP:HH2  | 2.08                     | 0.52              |
| 49:BQ:137:TYR:HE1 | 58:BZ:81:ARG:CZ   | 2.22                     | 0.52              |
| 51:BS:17:ARG:NH2  | 51:BS:90:GLY:H    | 2.07                     | 0.52              |
| 1:AA:1116:C:C2'   | 1:AA:1117:G:H5''  | 2.38                     | 0.52              |
| 1:AA:1287:A:N6    | 1:AA:1288:A:N6    | 2.58                     | 0.52              |
| 1:AA:1390:U:H6    | 1:AA:1390:U:O5'   | 1.92                     | 0.52              |
| 1:AA:186:C:H2'    | 1:AA:187:C:C5     | 2.44                     | 0.52              |
| 1:AA:346:G:H5''   | 52:BT:35:LYS:NZ   | 2.23                     | 0.52              |
| 1:AA:397:A:H5'    | 1:AA:398:C:OP1    | 2.09                     | 0.52              |
| 1:AA:699:C:H2'    | 1:AA:700:G:C5'    | 2.25                     | 0.52              |
| 1:AA:950:U:O2'    | 1:AA:951:G:C5'    | 2.57                     | 0.52              |
| 8:AH:58:TYR:O     | 8:AH:59:LEU:HD23  | 2.09                     | 0.52              |
| 9:AI:114:TYR:CE1  | 10:AJ:59:SER:HA   | 2.45                     | 0.52              |
| 9:AI:62:TYR:CE2   | 9:AI:64:THR:OG1   | 2.63                     | 0.52              |
| 10:AJ:35:SER:O    | 10:AJ:36:GLY:O    | 2.28                     | 0.52              |
| 19:AS:47:HIS:O    | 19:AS:62:ILE:HG23 | 2.09                     | 0.52              |
| 20:AT:89:ARG:NH2  | 20:AT:106:ALA:HB2 | 2.24                     | 0.52              |
| 24:AY:24:GLY:O    | 24:AY:28:THR:N    | 2.25                     | 0.52              |
| 26:B1:57:GLU:CG   | 26:B1:58:ILE:N    | 2.61                     | 0.52              |
| 29:B4:68:ARG:CD   | 29:B4:71:ARG:HD3  | 2.36                     | 0.52              |
| 31:B6:29:ASN:O    | 31:B6:30:THR:C    | 2.48                     | 0.52              |
| 35:BA:2206:G:H5'' | 35:BA:2207:G:OP2  | 2.08                     | 0.52              |
| 35:BA:2818:G:O2'  | 35:BA:2819:G:H5'  | 2.10                     | 0.52              |
| 35:BA:41:C:N4     | 35:BA:437:G:H1    | 2.07                     | 0.52              |
| 35:BA:926:A:H5'   | 35:BA:926:A:H8    | 1.73                     | 0.52              |
| 37:BC:171:ALA:HB1 | 37:BC:173:HIS:CE1 | 2.43                     | 0.52              |
| 42:BH:5:GLY:HA2   | 42:BH:69:ARG:HD3  | 1.91                     | 0.52              |
| 44:BK:57:UNK:HA   | 44:BK:67:UNK:N    | 2.24                     | 0.52              |
| 48:BP:23:PRO:C    | 48:BP:33:ARG:HE   | 2.12                     | 0.52              |
| 48:BP:88:LEU:HD11 | 48:BP:95:VAL:CG2  | 2.26                     | 0.52              |
| 51:BS:12:PHE:CD1  | 51:BS:12:PHE:C    | 2.82                     | 0.52              |
| 52:BT:38:ASN:N    | 52:BT:38:ASN:HD22 | 2.07                     | 0.52              |
| 54:BV:4:ILE:HD12  | 54:BV:40:LEU:HG   | 1.90                     | 0.52              |
| 54:BV:6:LYS:O     | 54:BV:37:VAL:HG21 | 2.09                     | 0.52              |
| 55:BW:90:ARG:NH1  | 55:BW:90:ARG:HG3  | 2.24                     | 0.52              |
| 58:BZ:3:TYR:N     | 58:BZ:3:TYR:CD1   | 2.78                     | 0.52              |
| 1:AA:1075:C:O2'   | 1:AA:1076:C:H5'   | 2.10                     | 0.52              |
| 1:AA:302:G:N3     | 1:AA:556:C:H4'    | 2.25                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:355:C:O4'     | 1:AA:388:G:O2'     | 2.26                     | 0.52              |
| 1:AA:493:G:H2'     | 1:AA:494:U:C5      | 2.45                     | 0.52              |
| 1:AA:543:C:H6      | 1:AA:543:C:O5'     | 1.92                     | 0.52              |
| 1:AA:625:G:H2'     | 1:AA:626:U:H6      | 1.74                     | 0.52              |
| 3:AC:74:GLY:O      | 3:AC:78:GLY:HA2    | 2.09                     | 0.52              |
| 24:AY:281:PRO:HB2  | 24:AY:286:ILE:HD13 | 1.92                     | 0.52              |
| 24:AY:61:ARG:NH2   | 24:AY:460:GLU:OE1  | 2.41                     | 0.52              |
| 30:B5:17:ASP:HB3   | 35:BA:16:G:OP1     | 2.09                     | 0.52              |
| 35:BA:142:A:H5'    | 35:BA:142(A):C:OP2 | 2.10                     | 0.52              |
| 35:BA:1484:G:H2'   | 35:BA:1485:G:C5'   | 2.22                     | 0.52              |
| 35:BA:1570:A:H2'   | 35:BA:1571:A:C8    | 2.44                     | 0.52              |
| 35:BA:1848:A:H2'   | 35:BA:1849:G:O4'   | 2.10                     | 0.52              |
| 35:BA:212:G:O2'    | 35:BA:213:A:H5'    | 2.10                     | 0.52              |
| 35:BA:35:G:O6      | 35:BA:446:G:N2     | 2.43                     | 0.52              |
| 42:BH:83:TYR:CB    | 42:BH:134:SER:HA   | 2.35                     | 0.52              |
| 42:BH:13:LYS:O     | 42:BH:15:VAL:N     | 2.42                     | 0.52              |
| 42:BH:149:ARG:NH1  | 42:BH:167:GLU:OE1  | 2.43                     | 0.52              |
| 35:BA:1048:A:H62   | 42:BH:1:MET:CE     | 2.22                     | 0.52              |
| 51:BS:22:GLY:O     | 51:BS:23:ARG:HB2   | 2.09                     | 0.52              |
| 51:BS:66:ALA:HB1   | 51:BS:99:LYS:CG    | 2.40                     | 0.52              |
| 54:BV:99:ILE:HD13  | 54:BV:99:ILE:N     | 2.24                     | 0.52              |
| 58:BZ:119:GLU:HG3  | 58:BZ:122:ARG:NH1  | 2.25                     | 0.52              |
| 1:AA:1030:C:C4'    | 1:AA:1030(A):G:H5' | 2.38                     | 0.52              |
| 1:AA:1066:C:H5'    | 1:AA:1067:A:OP2    | 2.09                     | 0.52              |
| 1:AA:697:U:C2'     | 1:AA:698:G:C5'     | 2.80                     | 0.52              |
| 3:AC:47:LEU:HD11   | 3:AC:87:LEU:HD13   | 1.90                     | 0.52              |
| 8:AH:30:ARG:HB3    | 8:AH:30:ARG:NH1    | 2.25                     | 0.52              |
| 9:AI:20:ARG:O      | 9:AI:60:ASP:N      | 2.41                     | 0.52              |
| 9:AI:88:TYR:O      | 9:AI:89:ASN:HB3    | 2.10                     | 0.52              |
| 11:AK:23:ALA:HB2   | 11:AK:28:THR:HG23  | 1.92                     | 0.52              |
| 13:AM:46:LYS:O     | 13:AM:46:LYS:HG2   | 2.09                     | 0.52              |
| 13:AM:74:VAL:O     | 13:AM:78:ILE:HG12  | 2.09                     | 0.52              |
| 15:AO:56:LEU:O     | 15:AO:60:VAL:HG23  | 2.10                     | 0.52              |
| 16:AP:59:TRP:HA    | 16:AP:62:VAL:CG2   | 2.39                     | 0.52              |
| 24:AY:437:THR:HG23 | 24:AY:454:MET:HG2  | 1.92                     | 0.52              |
| 24:AY:526:VAL:HB   | 24:AY:566:THR:CA   | 2.34                     | 0.52              |
| 24:AY:624:LEU:HD11 | 24:AY:655:TYR:OH   | 2.09                     | 0.52              |
| 27:B2:4:SER:C      | 27:B2:6:VAL:H      | 2.12                     | 0.52              |
| 29:B4:46:GLN:C     | 29:B4:48:ARG:H     | 2.10                     | 0.52              |
| 35:BA:1121:C:C2    | 35:BA:1122:G:C8    | 2.98                     | 0.52              |
| 35:BA:1149:G:H2'   | 35:BA:1150:C:C6    | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1424:G:C2'   | 35:BA:1425:G:O5'   | 2.58                     | 0.52              |
| 35:BA:1568:G:C5'   | 38:BD:61:LEU:HD23  | 2.39                     | 0.52              |
| 35:BA:195:A:H61    | 35:BA:198:C:H3'    | 1.75                     | 0.52              |
| 35:BA:2543:G:H2'   | 35:BA:2544:G:C8    | 2.43                     | 0.52              |
| 35:BA:2580:U:H4'   | 39:BE:130:GLY:HA3  | 1.91                     | 0.52              |
| 35:BA:271(L):U:C5' | 35:BA:271(M):G:H5' | 2.29                     | 0.52              |
| 35:BA:2777:G:H5''  | 35:BA:2778:A:C5'   | 2.40                     | 0.52              |
| 35:BA:812:C:O5'    | 48:BP:25:SER:HB2   | 2.09                     | 0.52              |
| 37:BC:109:MET:HA   | 37:BC:111:PHE:CE2  | 2.45                     | 0.52              |
| 39:BE:38:THR:HG21  | 39:BE:40:GLU:OE1   | 2.10                     | 0.52              |
| 40:BF:65:TRP:HZ3   | 40:BF:73:ALA:O     | 1.93                     | 0.52              |
| 41:BG:110:ALA:HB1  | 41:BG:142:PRO:CG   | 2.40                     | 0.52              |
| 42:BH:156:ALA:C    | 42:BH:158:HIS:H    | 2.11                     | 0.52              |
| 48:BP:6:LEU:HG     | 48:BP:9:ASN:CG     | 2.29                     | 0.52              |
| 49:BQ:29:PHE:HB3   | 49:BQ:65:PHE:CE2   | 2.44                     | 0.52              |
| 54:BV:2:PHE:CG     | 54:BV:13:ARG:NH1   | 2.77                     | 0.52              |
| 58:BZ:6:LYS:CD     | 58:BZ:6:LYS:N      | 2.72                     | 0.52              |
| 1:AA:1016:A:H2'    | 1:AA:1017:G:O4'    | 2.09                     | 0.52              |
| 1:AA:1306:A:N6     | 1:AA:1331:G:HO2'   | 2.08                     | 0.52              |
| 1:AA:359:U:H6      | 1:AA:359:U:O5'     | 1.91                     | 0.52              |
| 1:AA:415:A:O2'     | 1:AA:416:G:H5'     | 2.09                     | 0.52              |
| 1:AA:603:U:O2'     | 1:AA:604:G:H5'     | 2.10                     | 0.52              |
| 1:AA:992:U:H1'     | 1:AA:993:G:C2      | 2.45                     | 0.52              |
| 7:AG:80:VAL:HG12   | 7:AG:81:GLY:N      | 2.24                     | 0.52              |
| 10:AJ:61:GLU:OE2   | 14:AN:49:HIS:HE1   | 1.93                     | 0.52              |
| 12:AL:45:PRO:HG3   | 12:AL:53:ARG:CD    | 2.39                     | 0.52              |
| 24:AY:357:ARG:HG3  | 24:AY:357:ARG:HH11 | 1.74                     | 0.52              |
| 24:AY:487:ILE:CD1  | 24:AY:563:ILE:HG22 | 2.39                     | 0.52              |
| 26:B1:62:VAL:HG22  | 26:B1:63:ALA:N     | 2.25                     | 0.52              |
| 29:B4:23:GLU:O     | 29:B4:24:THR:C     | 2.48                     | 0.52              |
| 30:B5:19:ARG:NH1   | 35:BA:1265:A:H3'   | 2.24                     | 0.52              |
| 35:BA:1022:G:O6    | 46:BN:66:LYS:CE    | 2.57                     | 0.52              |
| 35:BA:1137:G:H2'   | 35:BA:1138:G:C8    | 2.44                     | 0.52              |
| 35:BA:1281:G:O2'   | 35:BA:1282:U:H5'   | 2.09                     | 0.52              |
| 35:BA:1405:U:H2'   | 35:BA:1406:U:H6    | 1.73                     | 0.52              |
| 35:BA:1820:U:O2'   | 38:BD:201:HIS:CD2  | 2.54                     | 0.52              |
| 35:BA:1993:U:H2'   | 35:BA:1994:C:C6    | 2.45                     | 0.52              |
| 35:BA:2176:A:C2'   | 35:BA:2177:C:C6    | 2.86                     | 0.52              |
| 35:BA:2376:A:H2'   | 35:BA:2377:A:O4'   | 2.09                     | 0.52              |
| 35:BA:2680:C:H2'   | 35:BA:2681:C:O2    | 2.09                     | 0.52              |
| 35:BA:1455:G:O6    | 35:BA:2705:A:C2    | 2.62                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:654(U):A:H2' | 35:BA:654(V):A:H8  | 1.75                     | 0.52              |
| 35:BA:747:U:O4     | 35:BA:2613:U:N3    | 2.42                     | 0.52              |
| 38:BD:69:ARG:NH2   | 38:BD:128:GLY:O    | 2.43                     | 0.52              |
| 40:BF:192:LEU:HD23 | 40:BF:193:VAL:N    | 2.25                     | 0.52              |
| 41:BG:135:LEU:HD12 | 41:BG:135:LEU:N    | 2.25                     | 0.52              |
| 41:BG:170:ARG:CZ   | 41:BG:180:PHE:HE2  | 2.22                     | 0.52              |
| 44:BK:99:UNK:O     | 44:BK:101:UNK:N    | 2.40                     | 0.52              |
| 48:BP:101:VAL:HA   | 48:BP:105:LEU:O    | 2.10                     | 0.52              |
| 57:BY:17:SER:HB3   | 57:BY:71:LYS:HB3   | 1.90                     | 0.52              |
| 1:AA:1306:A:H61    | 1:AA:1331:G:C1'    | 2.22                     | 0.52              |
| 1:AA:1320:C:H5''   | 19:AS:70:LYS:HG3   | 1.92                     | 0.52              |
| 1:AA:1331:G:OP2    | 13:AM:23:TYR:CD1   | 2.63                     | 0.52              |
| 1:AA:198:G:C5      | 1:AA:220:G:C2      | 2.96                     | 0.52              |
| 1:AA:346:G:C2'     | 1:AA:346:G:N3      | 2.73                     | 0.52              |
| 1:AA:495:A:O4'     | 1:AA:496:A:H5'     | 2.10                     | 0.52              |
| 1:AA:80:G:N3       | 1:AA:80:G:H2'      | 2.24                     | 0.52              |
| 6:AF:71:ARG:HH11   | 6:AF:71:ARG:HG3    | 1.75                     | 0.52              |
| 9:AI:106:ALA:O     | 9:AI:108:VAL:HG23  | 2.10                     | 0.52              |
| 9:AI:40:LEU:HD11   | 9:AI:70:LYS:HG2    | 1.92                     | 0.52              |
| 17:AQ:26:GLN:O     | 17:AQ:27:PHE:HB3   | 2.09                     | 0.52              |
| 18:AR:53:ARG:HA    | 18:AR:56:THR:OG1   | 2.10                     | 0.52              |
| 31:B6:45:LYS:O     | 31:B6:46:HIS:CB    | 2.58                     | 0.52              |
| 33:B8:28:GLY:O     | 33:B8:32:LEU:CD2   | 2.53                     | 0.52              |
| 35:BA:1420:U:H5'   | 35:BA:1421:G:OP2   | 2.09                     | 0.52              |
| 35:BA:1739:U:O2'   | 35:BA:1740:G:H5'   | 2.10                     | 0.52              |
| 25:B0:16:SER:HB2   | 35:BA:2262:U:H5    | 1.74                     | 0.52              |
| 35:BA:263:C:H2'    | 35:BA:264:C:C6     | 2.44                     | 0.52              |
| 35:BA:2747:G:O6    | 35:BA:2755:C:H5''  | 2.10                     | 0.52              |
| 35:BA:2853:C:H2'   | 35:BA:2854:G:H8    | 1.75                     | 0.52              |
| 35:BA:565:C:H4'    | 35:BA:1253:A:C6    | 2.45                     | 0.52              |
| 35:BA:603:A:H1'    | 35:BA:604:G:P      | 2.48                     | 0.52              |
| 36:BB:106:G:O2'    | 36:BB:107:G:H5'    | 2.09                     | 0.52              |
| 39:BE:132:HIS:CG   | 39:BE:135:HIS:NE2  | 2.77                     | 0.52              |
| 40:BF:77:ASP:O     | 40:BF:79:GLY:N     | 2.34                     | 0.52              |
| 41:BG:130:ASN:O    | 41:BG:159:VAL:HG13 | 2.09                     | 0.52              |
| 41:BG:48:GLU:CD    | 41:BG:49:ASP:N     | 2.62                     | 0.52              |
| 41:BG:83:ARG:N     | 41:BG:83:ARG:CD    | 2.69                     | 0.52              |
| 48:BP:101:VAL:CG1  | 48:BP:106:LEU:HD23 | 2.39                     | 0.52              |
| 49:BQ:58:PHE:O     | 49:BQ:58:PHE:HD1   | 1.91                     | 0.52              |
| 51:BS:106:ARG:NE   | 51:BS:108:GLY:HA3  | 2.25                     | 0.52              |
| 51:BS:12:PHE:HD1   | 51:BS:13:ARG:N     | 2.07                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:BU:85:LYS:NZ   | 53:BU:117:GLN:HE22 | 2.08                     | 0.52              |
| 57:BY:97:ARG:O    | 57:BY:98:VAL:HB    | 2.09                     | 0.52              |
| 1:AA:61:G:C6      | 1:AA:107:G:N1      | 2.78                     | 0.52              |
| 1:AA:1120:G:H2'   | 1:AA:1121:U:H6     | 1.75                     | 0.52              |
| 1:AA:1321:C:C5'   | 1:AA:1322:C:H5''   | 2.38                     | 0.52              |
| 1:AA:198:G:C6     | 1:AA:220:G:C4      | 2.98                     | 0.52              |
| 1:AA:793:U:OP2    | 1:AA:794:A:C8      | 2.63                     | 0.52              |
| 3:AC:188:LEU:HD12 | 3:AC:190:ARG:NH1   | 2.24                     | 0.52              |
| 6:AF:37:VAL:HG12  | 6:AF:38:GLU:N      | 2.24                     | 0.52              |
| 7:AG:36:LYS:O     | 7:AG:37:ASN:HB3    | 2.10                     | 0.52              |
| 13:AM:113:PRO:O   | 13:AM:114:ARG:HB2  | 2.09                     | 0.52              |
| 1:AA:750:G:N3     | 15:AO:23:GLY:HA3   | 2.25                     | 0.52              |
| 20:AT:27:LYS:HD3  | 20:AT:27:LYS:O     | 2.09                     | 0.52              |
| 22:AV:39:U:H6     | 22:AV:39:U:O5'     | 1.92                     | 0.52              |
| 24:AY:393:ASP:O   | 24:AY:394:ALA:O    | 2.28                     | 0.52              |
| 24:AY:487:ILE:CD1 | 24:AY:487:ILE:H    | 2.23                     | 0.52              |
| 25:B0:45:PHE:CZ   | 25:B0:77:ARG:NH2   | 2.77                     | 0.52              |
| 30:B5:16:ARG:HD2  | 30:B5:20:ARG:HH12  | 1.74                     | 0.52              |
| 35:BA:1223:G:N1   | 35:BA:1227:G:O6    | 2.41                     | 0.52              |
| 35:BA:413:C:H42   | 35:BA:2410:G:H1    | 1.57                     | 0.52              |
| 35:BA:260:G:O4'   | 35:BA:621:A:H1'    | 2.10                     | 0.52              |
| 35:BA:661:C:H4'   | 48:BP:16:ARG:NH1   | 2.23                     | 0.52              |
| 37:BC:44:VAL:HG21 | 37:BC:176:VAL:HG21 | 1.92                     | 0.52              |
| 39:BE:36:ARG:NH2  | 39:BE:88:GLY:CA    | 2.63                     | 0.52              |
| 41:BG:127:GLY:O   | 41:BG:129:GLY:N    | 2.43                     | 0.52              |
| 41:BG:89:GLY:O    | 41:BG:90:LEU:HB3   | 2.10                     | 0.52              |
| 42:BH:168:PRO:HB3 | 42:BH:170:ARG:NH2  | 2.25                     | 0.52              |
| 48:BP:9:ASN:N     | 48:BP:10:PRO:CD    | 2.72                     | 0.52              |
| 52:BT:30:VAL:CB   | 52:BT:31:SER:CB    | 2.69                     | 0.52              |
| 49:BQ:134:ARG:NH1 | 58:BZ:122:ARG:NH2  | 2.58                     | 0.52              |
| 58:BZ:98:MET:O    | 58:BZ:125:LEU:HA   | 2.09                     | 0.52              |
| 1:AA:1342:C:H2'   | 1:AA:1343:G:H8     | 1.74                     | 0.52              |
| 1:AA:1529:G:H2'   | 1:AA:1529:G:N3     | 2.25                     | 0.52              |
| 2:AB:77:ALA:HB2   | 2:AB:211:ILE:HD13  | 1.91                     | 0.52              |
| 4:AD:145:GLU:HG2  | 4:AD:184:LYS:HG2   | 1.92                     | 0.52              |
| 10:AJ:38:ILE:HG13 | 10:AJ:38:ILE:O     | 2.10                     | 0.52              |
| 20:AT:65:LYS:O    | 20:AT:68:LYS:HG2   | 2.10                     | 0.52              |
| 24:AY:327:PHE:CD1 | 24:AY:376:ALA:HB2  | 2.45                     | 0.52              |
| 26:B1:49:VAL:HG13 | 26:B1:49:VAL:O     | 2.09                     | 0.52              |
| 28:B3:4:LEU:HD11  | 28:B3:44:ARG:NE    | 2.25                     | 0.52              |
| 29:B4:16:CYS:SG   | 29:B4:21:VAL:HG21  | 2.50                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:B6:30:THR:O     | 31:B6:31:PRO:C    | 2.46                     | 0.52              |
| 35:BA:1486:A:C1'   | 35:BA:1505:C:H42  | 2.23                     | 0.52              |
| 35:BA:2105:C:OP1   | 35:BA:2105:C:O4'  | 2.27                     | 0.52              |
| 35:BA:2203:U:H3'   | 35:BA:2205:C:OP2  | 2.10                     | 0.52              |
| 35:BA:272(C):G:H2' | 35:BA:272(D):G:C8 | 2.45                     | 0.52              |
| 35:BA:316:C:C2'    | 35:BA:317:G:O5'   | 2.58                     | 0.52              |
| 35:BA:996:A:H4'    | 53:BU:92:ARG:HE   | 1.74                     | 0.52              |
| 37:BC:6:LYS:N      | 37:BC:9:ARG:NH1   | 2.58                     | 0.52              |
| 41:BG:55:LYS:HD3   | 41:BG:148:MET:CE  | 2.39                     | 0.52              |
| 41:BG:29:TRP:C     | 41:BG:31:VAL:H    | 2.13                     | 0.52              |
| 41:BG:77:ILE:HG21  | 41:BG:82:LEU:N    | 2.25                     | 0.52              |
| 41:BG:77:ILE:HD12  | 41:BG:80:PHE:CB   | 2.37                     | 0.52              |
| 42:BH:1:MET:O      | 42:BH:2:SER:OG    | 2.28                     | 0.52              |
| 42:BH:35:VAL:O     | 42:BH:37:VAL:HG23 | 2.10                     | 0.52              |
| 48:BP:30:THR:HA    | 48:BP:33:ARG:HD2  | 1.91                     | 0.52              |
| 51:BS:11:LYS:O     | 51:BS:11:LYS:HG2  | 2.10                     | 0.52              |
| 1:AA:268:C:O2'     | 1:AA:269:C:H5'    | 2.10                     | 0.52              |
| 1:AA:321:A:H62     | 1:AA:328:C:H1'    | 1.75                     | 0.52              |
| 1:AA:787:A:C2'     | 1:AA:788:U:H5'    | 2.40                     | 0.52              |
| 1:AA:797:C:O2'     | 1:AA:798:G:H5'    | 2.10                     | 0.52              |
| 1:AA:942:G:C2      | 1:AA:943:U:C4     | 2.98                     | 0.52              |
| 2:AB:212:GLN:NE2   | 2:AB:216:SER:OG   | 2.43                     | 0.52              |
| 3:AC:74:GLY:O      | 3:AC:78:GLY:N     | 2.43                     | 0.52              |
| 3:AC:90:GLU:HA     | 3:AC:93:LYS:HB2   | 1.91                     | 0.52              |
| 7:AG:51:GLN:O      | 7:AG:52:GLU:HB2   | 2.10                     | 0.52              |
| 14:AN:21:TYR:OH    | 14:AN:23:ARG:NH1  | 2.43                     | 0.52              |
| 24:AY:276:VAL:O    | 24:AY:280:LEU:HB2 | 2.10                     | 0.52              |
| 27:B2:48:HIS:CD2   | 27:B2:49:LYS:N    | 2.78                     | 0.52              |
| 27:B2:63:VAL:O     | 27:B2:66:GLU:CG   | 2.57                     | 0.52              |
| 32:B7:12:ARG:HD3   | 32:B7:46:VAL:CG2  | 2.40                     | 0.52              |
| 35:BA:1013:C:O2'   | 35:BA:1014:U:H5'  | 2.10                     | 0.52              |
| 35:BA:1151:G:H2'   | 35:BA:1152:C:C6   | 2.45                     | 0.52              |
| 35:BA:1445:A:H8    | 35:BA:1460:A:C4   | 2.28                     | 0.52              |
| 35:BA:1488:G:H5'   | 35:BA:1489:U:OP2  | 2.10                     | 0.52              |
| 35:BA:1579:A:H8    | 35:BA:1579:A:H5'  | 1.75                     | 0.52              |
| 35:BA:1892:C:C2'   | 35:BA:1893:C:C5'  | 2.72                     | 0.52              |
| 35:BA:1917:U:O2'   | 35:BA:1918:A:H5'  | 2.10                     | 0.52              |
| 35:BA:1925:C:H3'   | 35:BA:1926:U:H5'' | 1.91                     | 0.52              |
| 35:BA:1999:C:C2    | 35:BA:2000:G:C8   | 2.98                     | 0.52              |
| 35:BA:639:U:H2'    | 35:BA:640:C:C6    | 2.44                     | 0.52              |
| 36:BB:52:A:O2'     | 36:BB:53:A:C8     | 2.62                     | 0.52              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 35:BA:1258:C:O4'  | 40:BF:84:VAL:CG1    | 2.58                     | 0.52              |
| 42:BH:7:LEU:HD21  | 42:BH:69:ARG:HE     | 1.75                     | 0.52              |
| 49:BQ:141:GLN:HG3 | 58:BZ:72:ARG:CZ     | 2.40                     | 0.52              |
| 52:BT:34:VAL:HG22 | 52:BT:39:ARG:HA     | 1.91                     | 0.52              |
| 54:BV:81:TYR:C    | 54:BV:82:ARG:HD2    | 2.29                     | 0.52              |
| 57:BY:44:ILE:HD13 | 57:BY:65:ALA:HB2    | 1.91                     | 0.52              |
| 1:AA:1161:C:H2'   | 1:AA:1162:C:H6      | 1.75                     | 0.51              |
| 1:AA:1285:A:C1'   | 1:AA:1286:A:C8      | 2.93                     | 0.51              |
| 1:AA:1305:G:OP2   | 1:AA:1305:G:C8      | 2.63                     | 0.51              |
| 1:AA:1399:C:N3    | 1:AA:1502:A:N6      | 2.58                     | 0.51              |
| 1:AA:437:U:C2'    | 1:AA:438:G:H5'      | 2.40                     | 0.51              |
| 1:AA:506:G:H8     | 1:AA:506:G:O5'      | 1.92                     | 0.51              |
| 1:AA:663:A:O2'    | 1:AA:664:G:H5'      | 2.10                     | 0.51              |
| 1:AA:90:U:H4'     | 1:AA:91:C:OP1       | 2.09                     | 0.51              |
| 1:AA:91:C:O2      | 1:AA:91:C:C2'       | 2.57                     | 0.51              |
| 1:AA:982:U:H1'    | 1:AA:983:A:C2       | 2.44                     | 0.51              |
| 4:AD:182:LYS:HG2  | 4:AD:183:GLY:H      | 1.75                     | 0.51              |
| 6:AF:60:PHE:HE2   | 18:AR:76:LEU:HD12   | 1.75                     | 0.51              |
| 9:AI:2:GLU:O      | 9:AI:2:GLU:HG2      | 2.10                     | 0.51              |
| 12:AL:83:VAL:HG12 | 12:AL:84:LEU:N      | 2.24                     | 0.51              |
| 16:AP:28:ARG:HG2  | 16:AP:28:ARG:NH1    | 2.25                     | 0.51              |
| 19:AS:40:ILE:HG23 | 19:AS:67:VAL:C      | 2.30                     | 0.51              |
| 24:AY:96:ARG:HH11 | 24:AY:315:LYS:HG2   | 1.75                     | 0.51              |
| 24:AY:604:PRO:C   | 24:AY:605:ILE:HD12  | 2.31                     | 0.51              |
| 32:B7:45:ALA:O    | 32:B7:46:VAL:HG23   | 2.10                     | 0.51              |
| 33:B8:18:ALA:HB2  | 35:BA:628:G:O3'     | 2.10                     | 0.51              |
| 35:BA:1073:A:N3   | 35:BA:1073:A:H2'    | 2.24                     | 0.51              |
| 35:BA:1173:G:H3'  | 35:BA:1174:A:H5'    | 1.92                     | 0.51              |
| 35:BA:1221:C:O2'  | 35:BA:1221(A):C:H5' | 2.10                     | 0.51              |
| 35:BA:1381:G:O2'  | 35:BA:1382:G:H5'    | 2.10                     | 0.51              |
| 35:BA:1423:G:C2'  | 35:BA:1424:G:C5'    | 2.88                     | 0.51              |
| 35:BA:1697:G:H3'  | 35:BA:1698:A:C5'    | 2.37                     | 0.51              |
| 35:BA:1784:A:H4'  | 35:BA:1785:A:C5'    | 2.40                     | 0.51              |
| 35:BA:2404:C:C2'  | 35:BA:2405:G:O5'    | 2.58                     | 0.51              |
| 35:BA:935:C:H2'   | 35:BA:936:C:H6      | 1.75                     | 0.51              |
| 35:BA:960:A:H8    | 35:BA:960:A:O5'     | 1.93                     | 0.51              |
| 37:BC:100:ILE:C   | 37:BC:102:GLN:N     | 2.64                     | 0.51              |
| 37:BC:67:HIS:CG   | 37:BC:185:LYS:HD2   | 2.45                     | 0.51              |
| 37:BC:42:VAL:CG1  | 37:BC:43:GLU:N      | 2.73                     | 0.51              |
| 37:BC:48:LEU:CB   | 37:BC:50:ILE:HD12   | 2.38                     | 0.51              |
| 44:BK:25:UNK:O    | 44:BK:26:UNK:C      | 2.58                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:BP:108:LYS:HD2  | 48:BP:108:LYS:N    | 2.24                     | 0.51              |
| 51:BS:78:LEU:HD11  | 51:BS:103:GLU:CG   | 2.40                     | 0.51              |
| 51:BS:92:TYR:O     | 51:BS:93:LYS:CB    | 2.57                     | 0.51              |
| 51:BS:30:ARG:HH11  | 51:BS:97:ARG:CG    | 2.19                     | 0.51              |
| 57:BY:7:VAL:HB     | 57:BY:8:LYS:CE     | 2.40                     | 0.51              |
| 1:AA:119:A:H62     | 1:AA:287:U:H3      | 1.57                     | 0.51              |
| 1:AA:1211:U:H5'    | 1:AA:1212:U:OP1    | 2.09                     | 0.51              |
| 1:AA:1256:A:H2     | 1:AA:1277:C:C4     | 2.27                     | 0.51              |
| 1:AA:1495:U:O5'    | 1:AA:1495:U:H6     | 1.93                     | 0.51              |
| 1:AA:1499:A:C2     | 1:AA:1500:A:C8     | 2.99                     | 0.51              |
| 1:AA:1524:C:H2'    | 1:AA:1525:G:C8     | 2.45                     | 0.51              |
| 1:AA:197:A:O2'     | 1:AA:198:G:P       | 2.68                     | 0.51              |
| 1:AA:266:G:C5'     | 1:AA:267:C:C6      | 2.90                     | 0.51              |
| 1:AA:544:G:H2'     | 1:AA:545:C:O5'     | 2.09                     | 0.51              |
| 1:AA:580:U:H2'     | 1:AA:581:G:O4'     | 2.10                     | 0.51              |
| 1:AA:680:C:O2'     | 38:BD:166:GLN:HG2  | 2.10                     | 0.51              |
| 1:AA:796:C:H2'     | 1:AA:797:C:C6      | 2.43                     | 0.51              |
| 9:AI:126:SER:OG    | 9:AI:127:LYS:N     | 2.41                     | 0.51              |
| 11:AK:21:ILE:HG13  | 11:AK:30:VAL:HG12  | 1.91                     | 0.51              |
| 12:AL:26:ALA:O     | 12:AL:27:LEU:O     | 2.27                     | 0.51              |
| 13:AM:11:ARG:C     | 13:AM:13:LYS:N     | 2.64                     | 0.51              |
| 24:AY:386:GLY:HA2  | 24:AY:402:ILE:HG12 | 1.91                     | 0.51              |
| 12:AL:78:GLN:HE22  | 24:AY:444:PRO:HA   | 1.74                     | 0.51              |
| 24:AY:71:THR:HG22  | 24:AY:80:ASN:OD1   | 2.09                     | 0.51              |
| 35:BA:1992:G:C4    | 35:BA:1997:G:O6    | 2.63                     | 0.51              |
| 35:BA:2000:G:C2'   | 35:BA:2001:A:H5'   | 2.40                     | 0.51              |
| 35:BA:2103:C:H2'   | 35:BA:2104:G:H5'   | 1.92                     | 0.51              |
| 35:BA:2109:U:H1'   | 35:BA:2181:G:N2    | 2.24                     | 0.51              |
| 35:BA:2199:A:H5'   | 35:BA:2200:C:OP2   | 2.09                     | 0.51              |
| 35:BA:2320:A:C2    | 35:BA:2333:A:C8    | 2.98                     | 0.51              |
| 35:BA:2853:C:H2'   | 35:BA:2854:G:C8    | 2.46                     | 0.51              |
| 35:BA:654(E):G:O2' | 35:BA:654(F):C:H5' | 2.09                     | 0.51              |
| 36:BB:70:C:H2'     | 36:BB:71:C:H6      | 1.75                     | 0.51              |
| 37:BC:64:SER:HA    | 37:BC:161:ARG:H    | 1.74                     | 0.51              |
| 37:BC:29:LEU:O     | 37:BC:30:VAL:C     | 2.48                     | 0.51              |
| 40:BF:10:PRO:HA    | 40:BF:127:GLU:CG   | 2.40                     | 0.51              |
| 40:BF:139:PHE:CZ   | 40:BF:156:LEU:HD22 | 2.45                     | 0.51              |
| 40:BF:20:LEU:N     | 40:BF:24:LEU:HD21  | 2.25                     | 0.51              |
| 40:BF:28:ILE:HD13  | 40:BF:28:ILE:N     | 2.24                     | 0.51              |
| 42:BH:12:PRO:CD    | 42:BH:15:VAL:HG21  | 2.36                     | 0.51              |
| 44:BK:135:UNK:O    | 44:BK:137:UNK:N    | 2.44                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:BP:101:VAL:HG23 | 48:BP:102:ARG:N   | 2.24                     | 0.51              |
| 48:BP:111:ARG:HG3  | 48:BP:128:HIS:CG  | 2.45                     | 0.51              |
| 49:BQ:134:ARG:HA   | 49:BQ:137:TYR:CD2 | 2.43                     | 0.51              |
| 53:BU:83:LEU:HG    | 53:BU:88:ILE:HD11 | 1.92                     | 0.51              |
| 58:BZ:54:HIS:HB3   | 58:BZ:101:PRO:HD3 | 1.92                     | 0.51              |
| 1:AA:1499:A:H2'    | 1:AA:1500:A:H8    | 1.75                     | 0.51              |
| 1:AA:509:A:H3'     | 1:AA:509:A:P      | 2.50                     | 0.51              |
| 1:AA:662:G:H2'     | 1:AA:663:A:C8     | 2.45                     | 0.51              |
| 1:AA:81:U:H3'      | 1:AA:81:U:O2      | 2.10                     | 0.51              |
| 1:AA:833:U:H2'     | 1:AA:834:C:H6     | 1.75                     | 0.51              |
| 3:AC:22:TRP:HZ3    | 3:AC:24:ALA:CB    | 2.22                     | 0.51              |
| 18:AR:53:ARG:C     | 18:AR:55:ARG:H    | 2.13                     | 0.51              |
| 26:B1:4:VAL:HG23   | 26:B1:11:ARG:HG3  | 1.91                     | 0.51              |
| 27:B2:38:GLN:HA    | 27:B2:41:ILE:HD11 | 1.91                     | 0.51              |
| 35:BA:1029:A:O5'   | 35:BA:1029:A:H8   | 1.93                     | 0.51              |
| 35:BA:107:C:C2'    | 35:BA:108:U:H5'   | 2.40                     | 0.51              |
| 35:BA:1213:A:H2'   | 35:BA:1214:A:H8   | 1.76                     | 0.51              |
| 35:BA:1213:A:H2'   | 35:BA:1214:A:C8   | 2.45                     | 0.51              |
| 35:BA:1588:C:H2'   | 35:BA:1588:C:O2   | 2.10                     | 0.51              |
| 35:BA:1926:U:H2'   | 35:BA:1926:U:O2   | 2.10                     | 0.51              |
| 35:BA:2404:C:N4    | 35:BA:2414:G:C6   | 2.78                     | 0.51              |
| 37:BC:101:ILE:O    | 37:BC:103:LYS:N   | 2.42                     | 0.51              |
| 38:BD:21:PHE:HB3   | 38:BD:24:ILE:HG21 | 1.93                     | 0.51              |
| 39:BE:26:ILE:HG22  | 39:BE:27:LEU:N    | 2.24                     | 0.51              |
| 39:BE:47:VAL:HB    | 39:BE:49:LEU:CD2  | 2.40                     | 0.51              |
| 41:BG:35:GLU:O     | 41:BG:95:ARG:HB3  | 2.10                     | 0.51              |
| 42:BH:136:ILE:HD12 | 42:BH:136:ILE:H   | 1.75                     | 0.51              |
| 47:BO:13:ASN:ND2   | 47:BO:13:ASN:H    | 2.09                     | 0.51              |
| 48:BP:52:GLU:CG    | 48:BP:57:THR:HB   | 2.38                     | 0.51              |
| 55:BW:40:ASN:O     | 55:BW:41:LYS:HD3  | 2.10                     | 0.51              |
| 58:BZ:136:PHE:O    | 58:BZ:136:PHE:CD1 | 2.63                     | 0.51              |
| 1:AA:1151:A:C5     | 1:AA:1152:A:N6    | 2.78                     | 0.51              |
| 1:AA:1291:G:OP1    | 7:AG:37:ASN:ND2   | 2.42                     | 0.51              |
| 1:AA:490:G:N3      | 1:AA:491:G:C8     | 2.79                     | 0.51              |
| 3:AC:167:TRP:CD1   | 3:AC:167:TRP:C    | 2.83                     | 0.51              |
| 4:AD:208:SER:O     | 4:AD:209:ARG:HB2  | 2.09                     | 0.51              |
| 7:AG:15:ASP:CB     | 7:AG:19:GLY:O     | 2.52                     | 0.51              |
| 7:AG:38:LEU:C      | 7:AG:38:LEU:HD13  | 2.31                     | 0.51              |
| 10:AJ:51:ARG:HG3   | 10:AJ:60:ARG:CA   | 2.40                     | 0.51              |
| 11:AK:21:ILE:HD12  | 11:AK:21:ILE:N    | 2.26                     | 0.51              |
| 13:AM:80:ARG:HG3   | 19:AS:65:ASN:HD21 | 1.76                     | 0.51              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 15:AO:39:LEU:HD13  | 15:AO:56:LEU:HD23   | 1.91                     | 0.51              |
| 16:AP:34:GLU:OE1   | 16:AP:55:ARG:NH1    | 2.44                     | 0.51              |
| 22:AV:61:C:H2'     | 22:AV:62:C:H6       | 1.76                     | 0.51              |
| 24:AY:10:LYS:HA    | 24:AY:282:SER:OG    | 2.10                     | 0.51              |
| 24:AY:345:THR:HG22 | 24:AY:345:THR:O     | 2.11                     | 0.51              |
| 24:AY:507:TYR:HD1  | 24:AY:508:GLY:N     | 2.08                     | 0.51              |
| 24:AY:69:VAL:CA    | 24:AY:82:ILE:CG1    | 2.84                     | 0.51              |
| 26:B1:5:CYS:SG     | 26:B1:8:SER:HB3     | 2.51                     | 0.51              |
| 31:B6:42:TRP:CE3   | 31:B6:42:TRP:HA     | 2.46                     | 0.51              |
| 35:BA:1139:G:O2'   | 35:BA:1140:C:H5'    | 2.10                     | 0.51              |
| 35:BA:1142:U:H2'   | 35:BA:1142(A):A:OP1 | 2.10                     | 0.51              |
| 35:BA:1177:A:H4'   | 35:BA:1178:C:C5     | 2.45                     | 0.51              |
| 35:BA:1215:G:H2'   | 35:BA:1216:G:H8     | 1.76                     | 0.51              |
| 35:BA:1223:G:C6    | 35:BA:1227:G:C6     | 2.98                     | 0.51              |
| 35:BA:1643:G:C2    | 35:BA:1644:C:C2     | 2.99                     | 0.51              |
| 35:BA:2138:C:N4    | 35:BA:2153:G:O6     | 2.43                     | 0.51              |
| 35:BA:2713:A:C3'   | 35:BA:2714:G:H5'    | 2.26                     | 0.51              |
| 35:BA:494:G:OP1    | 55:BW:8:ARG:NH1     | 2.41                     | 0.51              |
| 38:BD:30:GLU:CG    | 38:BD:63:ARG:HH21   | 2.23                     | 0.51              |
| 40:BF:20:LEU:HD23  | 40:BF:21:ALA:N      | 2.23                     | 0.51              |
| 40:BF:7:TYR:CD2    | 40:BF:16:GLY:HA3    | 2.45                     | 0.51              |
| 40:BF:83:PHE:O     | 40:BF:86:GLY:N      | 2.35                     | 0.51              |
| 41:BG:82:LEU:HD22  | 41:BG:88:ILE:HD11   | 1.91                     | 0.51              |
| 41:BG:94:LEU:N     | 41:BG:94:LEU:CD2    | 2.74                     | 0.51              |
| 42:BH:20:ALA:HB1   | 42:BH:21:PRO:CD     | 2.40                     | 0.51              |
| 48:BP:95:VAL:CG2   | 48:BP:125:VAL:HG23  | 2.39                     | 0.51              |
| 35:BA:662:G:OP1    | 48:BP:18:ARG:CZ     | 2.59                     | 0.51              |
| 25:B0:4:LYS:HD2    | 49:BQ:82:ARG:CZ     | 2.40                     | 0.51              |
| 50:BR:2:ARG:C      | 50:BR:2:ARG:CD      | 2.79                     | 0.51              |
| 50:BR:2:ARG:O      | 50:BR:3:HIS:ND1     | 2.44                     | 0.51              |
| 51:BS:68:GLN:C     | 51:BS:70:GLY:H      | 2.14                     | 0.51              |
| 51:BS:93:LYS:O     | 51:BS:94:TYR:C      | 2.47                     | 0.51              |
| 57:BY:97:ARG:O     | 57:BY:98:VAL:HG23   | 2.10                     | 0.51              |
| 1:AA:1496:C:H2'    | 1:AA:1497:G:O4'     | 2.11                     | 0.51              |
| 1:AA:1392:G:N2     | 1:AA:1502:A:C8      | 2.79                     | 0.51              |
| 1:AA:310:G:H2'     | 1:AA:311:C:C6       | 2.45                     | 0.51              |
| 1:AA:60:A:N6       | 1:AA:110:C:N3       | 2.58                     | 0.51              |
| 1:AA:771:G:C5      | 1:AA:772:U:C5       | 2.98                     | 0.51              |
| 1:AA:868:C:H2'     | 1:AA:869:G:O5'      | 2.11                     | 0.51              |
| 4:AD:152:SER:O     | 4:AD:155:LEU:HB2    | 2.11                     | 0.51              |
| 6:AF:3:ARG:HB3     | 6:AF:93:SER:HB3     | 1.92                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:AG:57:GLU:O      | 7:AG:57:GLU:HG3   | 2.10                     | 0.51              |
| 9:AI:48:GLU:N      | 9:AI:49:PRO:CD    | 2.74                     | 0.51              |
| 9:AI:82:ALA:O      | 9:AI:86:VAL:HB    | 2.11                     | 0.51              |
| 9:AI:95:LYS:HD2    | 9:AI:96:LEU:N     | 2.25                     | 0.51              |
| 17:AQ:9:VAL:CG1    | 17:AQ:56:VAL:HG22 | 2.31                     | 0.51              |
| 22:AV:23:A:H2'     | 22:AV:24:G:H5'    | 1.92                     | 0.51              |
| 24:AY:165:GLN:HE21 | 24:AY:177:ILE:CG2 | 2.21                     | 0.51              |
| 26:B1:51:VAL:N     | 26:B1:58:ILE:O    | 2.35                     | 0.51              |
| 29:B4:10:VAL:CG2   | 29:B4:11:PRO:HD2  | 2.40                     | 0.51              |
| 35:BA:127:A:H5''   | 35:BA:128:C:O4'   | 2.10                     | 0.51              |
| 35:BA:15:G:C2      | 35:BA:16:G:C8     | 2.99                     | 0.51              |
| 35:BA:52:A:H2'     | 35:BA:53:A:H5'    | 1.92                     | 0.51              |
| 35:BA:960:A:H5''   | 35:BA:961:C:OP2   | 2.10                     | 0.51              |
| 37:BC:42:VAL:HG13  | 37:BC:43:GLU:H    | 1.73                     | 0.51              |
| 37:BC:68:GLY:H     | 37:BC:189:ASN:ND2 | 2.09                     | 0.51              |
| 39:BE:67:PHE:CD1   | 39:BE:69:LYS:HE3  | 2.45                     | 0.51              |
| 41:BG:135:LEU:C    | 41:BG:137:GLU:H   | 2.11                     | 0.51              |
| 41:BG:145:THR:HG22 | 41:BG:145:THR:O   | 2.10                     | 0.51              |
| 41:BG:7:LEU:CD2    | 41:BG:7:LEU:C     | 2.79                     | 0.51              |
| 43:BJ:90:UNK:O     | 43:BJ:91:UNK:C    | 2.58                     | 0.51              |
| 46:BN:39:ARG:HH21  | 46:BN:41:ASP:HB2  | 1.73                     | 0.51              |
| 46:BN:58:ASP:HB3   | 46:BN:95:PRO:HB2  | 1.91                     | 0.51              |
| 48:BP:147:LEU:O    | 48:BP:148:LEU:HB2 | 2.11                     | 0.51              |
| 51:BS:27:SER:HA    | 51:BS:88:ASP:HB3  | 1.93                     | 0.51              |
| 54:BV:64:HIS:ND1   | 54:BV:92:THR:CG2  | 2.71                     | 0.51              |
| 1:AA:1175:G:C2'    | 1:AA:1176:A:C5'   | 2.86                     | 0.51              |
| 1:AA:1395:C:H2'    | 1:AA:1396:A:H5'   | 1.93                     | 0.51              |
| 1:AA:324:G:N2      | 1:AA:326:G:H3'    | 2.26                     | 0.51              |
| 1:AA:347:G:N3      | 1:AA:348:G:C8     | 2.78                     | 0.51              |
| 1:AA:688:G:C5      | 1:AA:700:G:C2     | 2.98                     | 0.51              |
| 2:AB:76:GLN:O      | 2:AB:77:ALA:CB    | 2.58                     | 0.51              |
| 3:AC:84:ILE:C      | 3:AC:86:VAL:N     | 2.64                     | 0.51              |
| 4:AD:199:ASN:OD1   | 4:AD:201:GLN:HB2  | 2.11                     | 0.51              |
| 6:AF:90:VAL:HG13   | 6:AF:90:VAL:O     | 2.09                     | 0.51              |
| 8:AH:29:SER:HB3    | 8:AH:32:LYS:HG3   | 1.93                     | 0.51              |
| 8:AH:2:LEU:HD21    | 8:AH:5:PRO:HA     | 1.92                     | 0.51              |
| 9:AI:9:ARG:CG      | 9:AI:14:VAL:HG13  | 2.40                     | 0.51              |
| 13:AM:2:ALA:N      | 13:AM:9:ILE:CG2   | 2.74                     | 0.51              |
| 24:AY:401:SER:O    | 24:AY:402:ILE:CG1 | 2.59                     | 0.51              |
| 24:AY:491:VAL:HG12 | 24:AY:492:ASP:N   | 2.25                     | 0.51              |
| 25:B0:53:MET:CE    | 25:B0:57:PHE:CD2  | 2.94                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:B2:39:ALA:O     | 27:B2:42:GLY:N     | 2.41                     | 0.51              |
| 35:BA:1121:C:O5'   | 35:BA:1121:C:H6    | 1.93                     | 0.51              |
| 35:BA:1676:A:H2'   | 35:BA:1677:A:O4'   | 2.11                     | 0.51              |
| 35:BA:1876:A:H2'   | 35:BA:1877:A:C8    | 2.45                     | 0.51              |
| 35:BA:1941:C:O2'   | 35:BA:1942:C:H5'   | 2.10                     | 0.51              |
| 35:BA:320:A:H4'    | 35:BA:322:A:N7     | 2.25                     | 0.51              |
| 35:BA:330:A:H2     | 35:BA:1210:A:C2'   | 2.14                     | 0.51              |
| 35:BA:35:G:H2'     | 35:BA:36:G:H8      | 1.76                     | 0.51              |
| 35:BA:444:C:O2'    | 35:BA:445:C:H5'    | 2.09                     | 0.51              |
| 35:BA:601:C:H2'    | 35:BA:602:G:O4'    | 2.10                     | 0.51              |
| 35:BA:833:U:H2'    | 35:BA:834:C:C6     | 2.46                     | 0.51              |
| 35:BA:881:G:H2'    | 35:BA:882:G:O4'    | 2.10                     | 0.51              |
| 38:BD:70:TRP:CZ3   | 38:BD:150:LYS:HA   | 2.46                     | 0.51              |
| 35:BA:2632:A:O2'   | 39:BE:61:ARG:NH2   | 2.43                     | 0.51              |
| 39:BE:71:GLY:O     | 39:BE:73:GLU:N     | 2.43                     | 0.51              |
| 41:BG:36:LYS:HD3   | 41:BG:38:VAL:CG2   | 2.41                     | 0.51              |
| 42:BH:168:PRO:HB3  | 42:BH:170:ARG:HH21 | 1.76                     | 0.51              |
| 48:BP:111:ARG:HH11 | 48:BP:111:ARG:HG2  | 1.75                     | 0.51              |
| 48:BP:83:VAL:O     | 48:BP:83:VAL:HG13  | 2.11                     | 0.51              |
| 51:BS:51:ALA:CB    | 51:BS:73:LEU:HB2   | 2.41                     | 0.51              |
| 51:BS:51:ALA:HB3   | 51:BS:73:LEU:HB2   | 1.91                     | 0.51              |
| 55:BW:72:LYS:HD2   | 55:BW:106:ILE:HD11 | 1.92                     | 0.51              |
| 57:BY:2:ARG:CD     | 57:BY:3:VAL:HG23   | 2.40                     | 0.51              |
| 57:BY:7:VAL:C      | 57:BY:8:LYS:HD2    | 2.30                     | 0.51              |
| 57:BY:97:ARG:O     | 57:BY:98:VAL:CB    | 2.57                     | 0.51              |
| 1:AA:1126:U:OP2    | 1:AA:1281:U:O2     | 2.29                     | 0.51              |
| 1:AA:161:A:O2'     | 1:AA:162:A:H5'     | 2.08                     | 0.51              |
| 1:AA:687:A:H1'     | 1:AA:688:G:P       | 2.49                     | 0.51              |
| 7:AG:47:CYS:O      | 7:AG:48:LYS:C      | 2.48                     | 0.51              |
| 8:AH:1:MET:H3      | 8:AH:1:MET:CE      | 2.24                     | 0.51              |
| 24:AY:478:LYS:HG3  | 24:AY:478:LYS:O    | 2.10                     | 0.51              |
| 24:AY:575:VAL:HG12 | 24:AY:575:VAL:O    | 2.10                     | 0.51              |
| 31:B6:6:ARG:CB     | 31:B6:6:ARG:HH11   | 2.23                     | 0.51              |
| 35:BA:1107:G:H4'   | 43:BJ:81:UNK:CA    | 2.39                     | 0.51              |
| 35:BA:1233:C:O2'   | 35:BA:1234:U:H5'   | 2.11                     | 0.51              |
| 35:BA:1248:G:P     | 40:BF:92:PRO:HG3   | 2.51                     | 0.51              |
| 35:BA:1462:C:O2'   | 35:BA:1463:C:H5'   | 2.11                     | 0.51              |
| 35:BA:1496:A:H8    | 35:BA:1577:C:O2'   | 1.93                     | 0.51              |
| 35:BA:1799:G:C3'   | 35:BA:1799:G:OP1   | 2.43                     | 0.51              |
| 35:BA:2012:G:H8    | 35:BA:2012:G:O5'   | 1.94                     | 0.51              |
| 38:BD:134:ARG:CZ   | 38:BD:135:PHE:CE1  | 2.94                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BF:132:VAL:O    | 40:BF:138:GLU:OE1  | 2.29                     | 0.51              |
| 41:BG:39:ILE:CD1   | 41:BG:157:ILE:HG12 | 2.35                     | 0.51              |
| 41:BG:43:LEU:CD1   | 41:BG:48:GLU:H     | 2.24                     | 0.51              |
| 47:BO:23:ARG:HG3   | 47:BO:24:VAL:N     | 2.25                     | 0.51              |
| 48:BP:95:VAL:HG23  | 48:BP:125:VAL:HG23 | 1.92                     | 0.51              |
| 50:BR:9:LYS:C      | 50:BR:10:LEU:CD2   | 2.75                     | 0.51              |
| 57:BY:42:VAL:O     | 57:BY:65:ALA:HB3   | 2.11                     | 0.51              |
| 1:AA:1521:G:H2'    | 1:AA:1522:U:C6     | 2.45                     | 0.51              |
| 1:AA:473:G:H2'     | 1:AA:474:G:H8      | 1.75                     | 0.51              |
| 2:AB:24:TRP:CZ3    | 2:AB:32:ILE:HD12   | 2.46                     | 0.51              |
| 3:AC:106:VAL:O     | 3:AC:107:GLN:C     | 2.48                     | 0.51              |
| 1:AA:1189:C:O3'    | 3:AC:5:ILE:HD12    | 2.10                     | 0.51              |
| 4:AD:30:LYS:C      | 4:AD:32:ALA:N      | 2.63                     | 0.51              |
| 1:AA:1147:C:O2     | 9:AI:16:ARG:CZ     | 2.59                     | 0.51              |
| 9:AI:95:LYS:NZ     | 9:AI:96:LEU:HD13   | 2.26                     | 0.51              |
| 1:AA:1228:C:O5'    | 13:AM:115:LYS:HB3  | 2.10                     | 0.51              |
| 16:AP:54:GLU:HA    | 16:AP:54:GLU:OE1   | 2.11                     | 0.51              |
| 24:AY:129:LYS:HA   | 24:AY:253:LEU:HD21 | 1.92                     | 0.51              |
| 24:AY:494:GLU:CB   | 24:AY:511:LYS:HG2  | 2.40                     | 0.51              |
| 25:B0:56:ASP:C     | 25:B0:58:THR:N     | 2.63                     | 0.51              |
| 31:B6:41:PRO:CD    | 31:B6:45:LYS:HA    | 2.39                     | 0.51              |
| 33:B8:32:LEU:CB    | 33:B8:36:LYS:HZ1   | 2.23                     | 0.51              |
| 35:BA:1022:G:C6    | 35:BA:1141:U:C4    | 2.99                     | 0.51              |
| 35:BA:1227:G:H2'   | 35:BA:1228:G:C8    | 2.37                     | 0.51              |
| 35:BA:1601:G:C6    | 35:BA:1602:U:C4    | 2.99                     | 0.51              |
| 35:BA:1827:C:H2'   | 35:BA:1828:G:H5'   | 1.92                     | 0.51              |
| 35:BA:1859:A:C2    | 35:BA:1884:A:H1'   | 2.45                     | 0.51              |
| 35:BA:1919:A:H2'   | 35:BA:1920:C:C5'   | 2.39                     | 0.51              |
| 35:BA:2591:C:H2'   | 35:BA:2592:G:C8    | 2.46                     | 0.51              |
| 35:BA:747:U:C4     | 35:BA:2613:U:O4    | 2.53                     | 0.51              |
| 35:BA:315:G:H2'    | 35:BA:316:C:C6     | 2.45                     | 0.51              |
| 35:BA:654(M):C:H2' | 35:BA:654(N):G:C8  | 2.45                     | 0.51              |
| 35:BA:896:A:H1'    | 58:BZ:176:PRO:HB3  | 1.92                     | 0.51              |
| 36:BB:94:C:O2'     | 36:BB:95:C:H5'     | 2.11                     | 0.51              |
| 39:BE:174:ASP:OD1  | 39:BE:175:VAL:N    | 2.39                     | 0.51              |
| 39:BE:69:LYS:O     | 39:BE:71:GLY:N     | 2.43                     | 0.51              |
| 42:BH:5:GLY:C      | 42:BH:65:HIS:HE1   | 2.14                     | 0.51              |
| 48:BP:101:VAL:HG12 | 48:BP:106:LEU:HD23 | 1.93                     | 0.51              |
| 48:BP:107:LYS:C    | 48:BP:109:GLY:H    | 2.14                     | 0.51              |
| 48:BP:84:ASN:HD22  | 48:BP:115:LEU:HD23 | 1.75                     | 0.51              |
| 48:BP:79:ARG:O     | 48:BP:110:TYR:HB3  | 2.10                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:BP:84:ASN:OD1   | 48:BP:116:GLY:CA  | 2.54                     | 0.51              |
| 50:BR:85:PRO:O     | 50:BR:87:TYR:N    | 2.44                     | 0.51              |
| 52:BT:95:ARG:HA    | 52:BT:95:ARG:HH11 | 1.76                     | 0.51              |
| 53:BU:80:ILE:O     | 53:BU:84:LYS:HB2  | 2.11                     | 0.51              |
| 53:BU:92:ARG:HB2   | 54:BV:11:GLN:NE2  | 2.24                     | 0.51              |
| 54:BV:21:ARG:HD3   | 54:BV:21:ARG:N    | 2.26                     | 0.51              |
| 55:BW:6:ILE:HA     | 55:BW:103:ILE:O   | 2.11                     | 0.51              |
| 57:BY:17:SER:HA    | 57:BY:71:LYS:HE2  | 1.93                     | 0.51              |
| 57:BY:99:CYS:O     | 57:BY:100:ALA:HB2 | 2.11                     | 0.51              |
| 58:BZ:108:PRO:HA   | 58:BZ:142:SER:HA  | 1.92                     | 0.51              |
| 58:BZ:183:LEU:HD11 | 58:BZ:186:GLU:CA  | 2.41                     | 0.51              |
| 1:AA:1412:C:H2'    | 1:AA:1413:A:C8    | 2.46                     | 0.51              |
| 1:AA:311:C:C3'     | 1:AA:312:C:H5'    | 2.30                     | 0.51              |
| 1:AA:322:C:H2'     | 1:AA:323:U:H5'    | 1.93                     | 0.51              |
| 1:AA:973:G:OP1     | 10:AJ:57:LYS:NZ   | 2.35                     | 0.51              |
| 4:AD:126:ILE:HG22  | 4:AD:127:THR:N    | 2.25                     | 0.51              |
| 9:AI:80:GLY:O      | 9:AI:81:ILE:C     | 2.49                     | 0.51              |
| 17:AQ:68:ARG:N     | 17:AQ:70:ARG:HH11 | 2.08                     | 0.51              |
| 22:AV:45:U:O2      | 22:AV:45:U:C3'    | 2.59                     | 0.51              |
| 24:AY:264:LEU:HB2  | 61:AY:701:GCP:N7  | 2.26                     | 0.51              |
| 26:B1:53:VAL:HG21  | 26:B1:58:ILE:CD1  | 2.38                     | 0.51              |
| 35:BA:1027:A:O2'   | 35:BA:1028:A:H5'  | 2.11                     | 0.51              |
| 35:BA:1188:U:O2'   | 35:BA:1189:A:H5'  | 2.10                     | 0.51              |
| 35:BA:1649:G:H2'   | 35:BA:1650:G:H5'  | 1.92                     | 0.51              |
| 35:BA:2181:G:O2'   | 35:BA:2182:G:H5'  | 2.11                     | 0.51              |
| 35:BA:2207:G:C5'   | 35:BA:2207:G:N3   | 2.64                     | 0.51              |
| 35:BA:2273:A:H2'   | 35:BA:2274:A:C8   | 2.46                     | 0.51              |
| 35:BA:264:C:O5'    | 35:BA:264:C:H6    | 1.92                     | 0.51              |
| 35:BA:2808:U:H5'   | 35:BA:2891:G:O6   | 2.10                     | 0.51              |
| 35:BA:7:G:H2'      | 35:BA:8:A:C8      | 2.46                     | 0.51              |
| 40:BF:101:LEU:HD12 | 40:BF:102:PRO:CD  | 2.40                     | 0.51              |
| 41:BG:106:LEU:HA   | 41:BG:110:ALA:CB  | 2.41                     | 0.51              |
| 41:BG:180:PHE:O    | 41:BG:181:ARG:O   | 2.29                     | 0.51              |
| 35:BA:2653:U:O2'   | 42:BH:110:SER:HB2 | 2.11                     | 0.51              |
| 42:BH:149:ARG:HA   | 42:BH:162:ILE:CG1 | 2.41                     | 0.51              |
| 42:BH:169:VAL:HG13 | 42:BH:170:ARG:H   | 1.75                     | 0.51              |
| 42:BH:26:VAL:O     | 42:BH:32:GLU:HA   | 2.10                     | 0.51              |
| 46:BN:90:MET:CE    | 46:BN:90:MET:HA   | 2.41                     | 0.51              |
| 48:BP:115:LEU:CD2  | 48:BP:116:GLY:N   | 2.74                     | 0.51              |
| 53:BU:74:LEU:CD1   | 53:BU:79:PHE:HB2  | 2.41                     | 0.51              |
| 53:BU:95:LEU:O     | 53:BU:98:LEU:HG   | 2.11                     | 0.51              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 53:BU:91:ASP:CG     | 53:BU:96:ALA:HB2   | 2.30                     | 0.51              |
| 57:BY:84:ARG:HH21   | 57:BY:97:ARG:HB3   | 1.76                     | 0.51              |
| 58:BZ:108:PRO:HG2   | 58:BZ:111:VAL:CG2  | 2.41                     | 0.51              |
| 58:BZ:28:MET:HE3    | 58:BZ:59:LEU:HD12  | 1.93                     | 0.51              |
| 1:AA:110:C:H2'      | 1:AA:111:G:C5'     | 2.40                     | 0.51              |
| 1:AA:1128:C:O2'     | 1:AA:1129:C:H5''   | 2.11                     | 0.51              |
| 1:AA:1316:G:H2'     | 1:AA:1317:C:H5''   | 1.93                     | 0.51              |
| 1:AA:157:G:H2'      | 1:AA:158:G:H8      | 1.75                     | 0.51              |
| 1:AA:388:G:O2'      | 1:AA:389:A:P       | 2.69                     | 0.51              |
| 1:AA:397:A:H3'      | 1:AA:397:A:N3      | 2.26                     | 0.51              |
| 1:AA:549:C:C2       | 1:AA:550:G:C8      | 2.99                     | 0.51              |
| 1:AA:555:C:H2'      | 1:AA:556:C:C5      | 2.46                     | 0.51              |
| 1:AA:560:U:C5'      | 1:AA:561:U:H3'     | 2.39                     | 0.51              |
| 1:AA:63:C:C5'       | 1:AA:64:G:OP2      | 2.54                     | 0.51              |
| 1:AA:868:C:C2'      | 1:AA:869:G:C5'     | 2.89                     | 0.51              |
| 4:AD:152:SER:HA     | 4:AD:155:LEU:HD12  | 1.93                     | 0.51              |
| 5:AE:51:VAL:O       | 5:AE:55:VAL:HG23   | 2.10                     | 0.51              |
| 5:AE:80:ILE:HG22    | 8:AH:104:ARG:NH2   | 2.26                     | 0.51              |
| 11:AK:79:SER:OG     | 11:AK:106:LYS:HD2  | 2.11                     | 0.51              |
| 17:AQ:59:ILE:HG22   | 17:AQ:71:PHE:CD2   | 2.46                     | 0.51              |
| 19:AS:6:LYS:CG      | 19:AS:7:LYS:H      | 2.12                     | 0.51              |
| 24:AY:512:ILE:H     | 24:AY:512:ILE:HD13 | 1.76                     | 0.51              |
| 24:AY:70:THR:O      | 24:AY:80:ASN:HA    | 2.11                     | 0.51              |
| 26:B1:29:GLY:O      | 26:B1:30:VAL:CB    | 2.58                     | 0.51              |
| 27:B2:50:ILE:CG2    | 27:B2:51:ARG:N     | 2.72                     | 0.51              |
| 35:BA:1180:C:C2'    | 35:BA:1181:C:H5'   | 2.41                     | 0.51              |
| 35:BA:1348:G:C2'    | 35:BA:1349:A:H5''  | 2.40                     | 0.51              |
| 35:BA:139(A):G:H3'  | 35:BA:140:G:H8     | 1.76                     | 0.51              |
| 35:BA:1854:A:H62    | 35:BA:1888:G:H8    | 1.59                     | 0.51              |
| 35:BA:213:A:O2'     | 35:BA:214:G:H5'    | 2.11                     | 0.51              |
| 35:BA:2648:C:H2'    | 35:BA:2649:U:C6    | 2.46                     | 0.51              |
| 35:BA:271(J):C:HO2' | 35:BA:271(K):U:H6  | 1.57                     | 0.51              |
| 37:BC:65:LEU:HB3    | 37:BC:189:ASN:HD22 | 1.75                     | 0.51              |
| 38:BD:26:LYS:NZ     | 38:BD:26:LYS:HA    | 2.25                     | 0.51              |
| 35:BA:779:U:OP1     | 38:BD:49:ILE:HG13  | 2.11                     | 0.51              |
| 41:BG:103:LEU:CD1   | 41:BG:107:LEU:HG   | 2.41                     | 0.51              |
| 41:BG:137:GLU:HG3   | 41:BG:155:MET:N    | 2.25                     | 0.51              |
| 41:BG:55:LYS:HD3    | 41:BG:148:MET:HE1  | 1.92                     | 0.51              |
| 42:BH:12:PRO:HD3    | 42:BH:76:VAL:HG13  | 1.92                     | 0.51              |
| 44:BK:28:UNK:O      | 44:BK:31:UNK:N     | 2.44                     | 0.51              |
| 45:BL:92:UNK:O      | 45:BL:94:UNK:N     | 2.43                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:627:A:H62    | 48:BP:84:ASN:HD21  | 1.59                     | 0.51              |
| 51:BS:20:ARG:NE    | 51:BS:20:ARG:HA    | 2.24                     | 0.51              |
| 51:BS:35:ILE:HD13  | 51:BS:99:LYS:HD3   | 1.92                     | 0.51              |
| 54:BV:18:LEU:O     | 54:BV:19:LYS:HB2   | 2.10                     | 0.51              |
| 55:BW:58:ALA:O     | 55:BW:64:MET:HG3   | 2.10                     | 0.51              |
| 56:BX:35:THR:CG2   | 56:BX:36:LYS:N     | 2.74                     | 0.51              |
| 58:BZ:44:PHE:CE1   | 58:BZ:48:PHE:HD2   | 2.29                     | 0.51              |
| 58:BZ:45:ASP:O     | 58:BZ:49:ARG:HG2   | 2.10                     | 0.51              |
| 1:AA:1116:C:C2'    | 1:AA:1117:G:C5'    | 2.89                     | 0.50              |
| 1:AA:1014:A:C2     | 1:AA:1219:U:H1'    | 2.46                     | 0.50              |
| 1:AA:77:G:N1       | 1:AA:92:C:N4       | 2.60                     | 0.50              |
| 2:AB:39:ILE:O      | 2:AB:41:ILE:HD13   | 2.10                     | 0.50              |
| 4:AD:126:ILE:CG2   | 4:AD:127:THR:N     | 2.73                     | 0.50              |
| 1:AA:511:C:O4'     | 4:AD:43:HIS:NE2    | 2.44                     | 0.50              |
| 4:AD:83:SER:HA     | 4:AD:89:THR:CG2    | 2.41                     | 0.50              |
| 6:AF:87:ARG:HG2    | 6:AF:87:ARG:HH11   | 1.77                     | 0.50              |
| 11:AK:121:PRO:HG2  | 11:AK:126:ARG:HG3  | 1.92                     | 0.50              |
| 24:AY:15:ILE:HD12  | 24:AY:81:ILE:HG23  | 1.94                     | 0.50              |
| 24:AY:38:ARG:NH2   | 24:AY:270:GLN:NE2  | 2.58                     | 0.50              |
| 25:B0:69:PHE:N     | 25:B0:69:PHE:HD1   | 2.08                     | 0.50              |
| 26:B1:63:ALA:O     | 26:B1:67:ILE:HG13  | 2.11                     | 0.50              |
| 26:B1:85:LEU:O     | 26:B1:86:SER:HB3   | 2.11                     | 0.50              |
| 31:B6:18:ARG:HH22  | 31:B6:44:ARG:HB3   | 1.76                     | 0.50              |
| 33:B8:15:LYS:HD2   | 48:BP:65:ARG:NH2   | 2.25                     | 0.50              |
| 33:B8:2:PRO:O      | 33:B8:3:LYS:C      | 2.49                     | 0.50              |
| 35:BA:1762:A:O5'   | 35:BA:1762:A:H8    | 1.93                     | 0.50              |
| 35:BA:17:G:H2'     | 35:BA:18:C:C5      | 2.45                     | 0.50              |
| 35:BA:1786:A:C4    | 35:BA:1938:A:C6    | 2.98                     | 0.50              |
| 35:BA:2180:U:H5'   | 35:BA:2180:U:C6    | 2.32                     | 0.50              |
| 35:BA:2339:G:H2'   | 35:BA:2340:G:H8    | 1.74                     | 0.50              |
| 35:BA:402:A:C2'    | 35:BA:403:U:H5'    | 2.42                     | 0.50              |
| 35:BA:436:C:H2'    | 35:BA:437:G:C8     | 2.47                     | 0.50              |
| 35:BA:953:A:N6     | 35:BA:965:C:C4     | 2.78                     | 0.50              |
| 35:BA:965:C:O2'    | 35:BA:966:G:H5'    | 2.11                     | 0.50              |
| 37:BC:138:LEU:HD23 | 37:BC:139:PRO:CD   | 2.41                     | 0.50              |
| 37:BC:191:ARG:O    | 37:BC:195:ARG:HG2  | 2.11                     | 0.50              |
| 37:BC:50:ILE:H     | 37:BC:50:ILE:HD13  | 1.76                     | 0.50              |
| 38:BD:69:ARG:CD    | 38:BD:105:ILE:HD11 | 2.34                     | 0.50              |
| 39:BE:6:GLY:O      | 39:BE:195:LEU:HD12 | 2.10                     | 0.50              |
| 40:BF:135:LYS:H    | 40:BF:166:ALA:CB   | 2.24                     | 0.50              |
| 42:BH:171:LEU:O    | 42:BH:173:PRO:CD   | 2.51                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BJ:96:UNK:C     | 43:BJ:98:UNK:N     | 2.74                     | 0.50              |
| 46:BN:85:ILE:HD12  | 46:BN:85:ILE:N     | 2.26                     | 0.50              |
| 35:BA:833:U:C4'    | 48:BP:51:PHE:O     | 2.59                     | 0.50              |
| 51:BS:24:LEU:CB    | 51:BS:85:VAL:HG12  | 2.41                     | 0.50              |
| 56:BX:83:VAL:HG12  | 56:BX:84:ALA:N     | 2.26                     | 0.50              |
| 58:BZ:97:GLU:HG3   | 58:BZ:127:LYS:CB   | 2.35                     | 0.50              |
| 1:AA:1152:A:C2     | 1:AA:1153:C:N3     | 2.79                     | 0.50              |
| 1:AA:1444:C:O2'    | 1:AA:1445:C:H5'    | 2.11                     | 0.50              |
| 1:AA:323:U:H2'     | 1:AA:324:G:O4'     | 2.11                     | 0.50              |
| 1:AA:514:C:H2'     | 1:AA:515:G:H8      | 1.75                     | 0.50              |
| 1:AA:769:G:C2'     | 1:AA:770:C:C5'     | 2.78                     | 0.50              |
| 2:AB:104:ASN:CG    | 2:AB:107:THR:HB    | 2.31                     | 0.50              |
| 3:AC:64:VAL:HG12   | 3:AC:66:VAL:CG2    | 2.41                     | 0.50              |
| 3:AC:95:THR:O      | 3:AC:97:LYS:N      | 2.38                     | 0.50              |
| 8:AH:122:ARG:CZ    | 8:AH:122:ARG:HB2   | 2.41                     | 0.50              |
| 9:AI:33:PHE:HD2    | 9:AI:34:ASN:ND2    | 2.09                     | 0.50              |
| 1:AA:963:G:N2      | 10:AJ:55:LYS:CE    | 2.75                     | 0.50              |
| 10:AJ:6:ILE:HB     | 10:AJ:98:ILE:HD12  | 1.94                     | 0.50              |
| 11:AK:124:LYS:HZ3  | 11:AK:125:PHE:HE1  | 1.57                     | 0.50              |
| 24:AY:11:ARG:HA    | 24:AY:77:HIS:CE1   | 2.46                     | 0.50              |
| 24:AY:463:VAL:O    | 24:AY:466:LEU:HB2  | 2.11                     | 0.50              |
| 33:B8:31:HIS:O     | 33:B8:32:LEU:C     | 2.48                     | 0.50              |
| 35:BA:1215:G:HO2'  | 35:BA:1216:G:H5'   | 1.66                     | 0.50              |
| 35:BA:1301:A:H2'   | 35:BA:1302:A:C3'   | 2.41                     | 0.50              |
| 35:BA:1788:C:O2'   | 35:BA:1789:A:H5'   | 2.10                     | 0.50              |
| 35:BA:2261:C:O2'   | 35:BA:2262:U:H5'   | 2.10                     | 0.50              |
| 35:BA:2691:C:H5'   | 35:BA:2691:C:H6    | 1.76                     | 0.50              |
| 35:BA:271(R):G:O2' | 35:BA:271(S):G:H5' | 2.11                     | 0.50              |
| 35:BA:637:A:H4'    | 35:BA:638:G:O5'    | 2.11                     | 0.50              |
| 35:BA:71:A:C2      | 56:BX:31:HIS:CE1   | 2.97                     | 0.50              |
| 35:BA:996:A:O2'    | 53:BU:92:ARG:HG3   | 2.11                     | 0.50              |
| 36:BB:30:C:H2'     | 36:BB:31:C:O4'     | 2.11                     | 0.50              |
| 40:BF:167:ALA:O    | 40:BF:169:ASN:N    | 2.44                     | 0.50              |
| 41:BG:16:ARG:HB3   | 41:BG:17:PRO:HD3   | 1.92                     | 0.50              |
| 41:BG:69:ALA:O     | 41:BG:90:LEU:HD12  | 2.11                     | 0.50              |
| 42:BH:11:VAL:HB    | 42:BH:48:GLY:O     | 2.12                     | 0.50              |
| 42:BH:39:PRO:C     | 42:BH:41:MET:H     | 2.14                     | 0.50              |
| 42:BH:9:ILE:HA     | 42:BH:69:ARG:NH1   | 2.26                     | 0.50              |
| 49:BQ:51:ARG:O     | 49:BQ:55:VAL:HG12  | 2.11                     | 0.50              |
| 35:BA:1453:U:H5'   | 50:BR:63:ARG:NE    | 2.26                     | 0.50              |
| 52:BT:121:ILE:O    | 52:BT:124:ASP:HB2  | 2.11                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 57:BY:81:LYS:HD3   | 57:BY:97:ARG:O    | 2.11                     | 0.50              |
| 1:AA:1285:A:HO2'   | 1:AA:1286:A:P     | 2.32                     | 0.50              |
| 1:AA:107:G:OP1     | 1:AA:325:A:N6     | 2.45                     | 0.50              |
| 1:AA:390:C:O3'     | 16:AP:28:ARG:NH2  | 2.44                     | 0.50              |
| 1:AA:775:G:H2'     | 1:AA:776:G:C5'    | 2.41                     | 0.50              |
| 1:AA:788:U:HO2'    | 23:AX:13:A:H2     | 1.57                     | 0.50              |
| 5:AE:80:ILE:HG13   | 5:AE:91:LEU:HB2   | 1.93                     | 0.50              |
| 10:AJ:38:ILE:CG1   | 10:AJ:71:LEU:HB3  | 2.41                     | 0.50              |
| 11:AK:58:PRO:O     | 11:AK:61:ALA:HB3  | 2.11                     | 0.50              |
| 13:AM:40:ASN:HB3   | 13:AM:43:THR:HG23 | 1.93                     | 0.50              |
| 22:AV:9:A:H62      | 22:AV:23:A:H2     | 1.60                     | 0.50              |
| 24:AY:616:TYR:CE2  | 24:AY:664:GLN:HG3 | 2.45                     | 0.50              |
| 35:BA:1023:U:C3'   | 35:BA:1024:G:H5'  | 2.38                     | 0.50              |
| 35:BA:109:G:C2     | 35:BA:110:G:C4    | 2.99                     | 0.50              |
| 35:BA:139(A):G:H3' | 35:BA:140:G:C8    | 2.47                     | 0.50              |
| 35:BA:1446:C:H5    | 35:BA:1466:G:C2   | 2.28                     | 0.50              |
| 35:BA:1544:A:H2'   | 35:BA:1545:A:C8   | 2.46                     | 0.50              |
| 35:BA:1773:A:N7    | 35:BA:1829:A:H1'  | 2.26                     | 0.50              |
| 35:BA:2009:G:N1    | 35:BA:2010:G:N7   | 2.59                     | 0.50              |
| 35:BA:2124:G:H2'   | 35:BA:2125:G:C5'  | 2.41                     | 0.50              |
| 35:BA:2305:A:C2    | 35:BA:2306:C:C1'  | 2.94                     | 0.50              |
| 35:BA:2606:C:C3'   | 35:BA:2607:G:H5'  | 2.41                     | 0.50              |
| 35:BA:2875:C:H4'   | 52:BT:5:ALA:HB2   | 1.93                     | 0.50              |
| 35:BA:527:C:O2     | 35:BA:527:C:H5'   | 2.12                     | 0.50              |
| 35:BA:692:C:H2'    | 35:BA:693:C:H6    | 1.75                     | 0.50              |
| 35:BA:699:A:C2'    | 35:BA:700:G:C5'   | 2.86                     | 0.50              |
| 27:B2:47:ASN:ND2   | 35:BA:95:G:H1'    | 2.25                     | 0.50              |
| 38:BD:146:GLU:HG2  | 38:BD:152:GLY:C   | 2.31                     | 0.50              |
| 39:BE:179:GLU:O    | 39:BE:180:ASN:HB2 | 2.11                     | 0.50              |
| 35:BA:1256:G:H21   | 40:BF:82:ILE:HG22 | 1.77                     | 0.50              |
| 42:BH:1:MET:HG3    | 42:BH:2:SER:N     | 2.26                     | 0.50              |
| 49:BQ:135:ASP:N    | 49:BQ:137:TYR:CD2 | 2.79                     | 0.50              |
| 49:BQ:12:GLN:OE1   | 49:BQ:72:LYS:HG3  | 2.11                     | 0.50              |
| 36:BB:49:C:OP1     | 51:BS:97:ARG:HG3  | 2.11                     | 0.50              |
| 57:BY:60:PHE:C     | 57:BY:61:ILE:HG13 | 2.32                     | 0.50              |
| 58:BZ:30:ASN:O     | 58:BZ:31:ARG:C    | 2.50                     | 0.50              |
| 58:BZ:32:HIS:O     | 58:BZ:33:LEU:HB3  | 2.11                     | 0.50              |
| 1:AA:1392:G:H21    | 1:AA:1502:A:H8    | 1.57                     | 0.50              |
| 1:AA:175:C:H2'     | 1:AA:176:C:H6     | 1.77                     | 0.50              |
| 3:AC:108:ASN:HB3   | 3:AC:111:LEU:HB2  | 1.93                     | 0.50              |
| 5:AE:100:VAL:O     | 5:AE:107:ARG:NH2  | 2.45                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:AJ:66:ARG:HH11  | 10:AJ:66:ARG:CB     | 2.25                     | 0.50              |
| 12:AL:27:LEU:O     | 12:AL:28:LYS:C      | 2.49                     | 0.50              |
| 1:AA:1049:U:H2'    | 14:AN:2:ALA:N       | 2.25                     | 0.50              |
| 14:AN:58:LYS:HZ2   | 14:AN:58:LYS:HB3    | 1.74                     | 0.50              |
| 16:AP:52:ASP:OD1   | 16:AP:54:GLU:HB2    | 2.12                     | 0.50              |
| 24:AY:141:LYS:HG2  | 24:AY:142:THR:N     | 2.27                     | 0.50              |
| 24:AY:211:GLU:O    | 24:AY:215:LYS:HG3   | 2.11                     | 0.50              |
| 25:B0:11:ARG:HD3   | 25:B0:12:ASN:N      | 2.17                     | 0.50              |
| 25:B0:11:ARG:O     | 25:B0:14:ARG:NH1    | 2.44                     | 0.50              |
| 26:B1:26:ARG:HG3   | 26:B1:27:GLU:N      | 2.21                     | 0.50              |
| 26:B1:75:GLU:C     | 26:B1:78:LYS:HD2    | 2.32                     | 0.50              |
| 26:B1:81:LYS:HE3   | 35:BA:271(H):G:H5'' | 1.92                     | 0.50              |
| 30:B5:40:LYS:HZ3   | 30:B5:46:CYS:HB3    | 1.72                     | 0.50              |
| 35:BA:1109:C:H2'   | 35:BA:1110:G:O4'    | 2.11                     | 0.50              |
| 35:BA:1025:G:C4    | 35:BA:1135:C:C1'    | 2.95                     | 0.50              |
| 35:BA:565:C:H4'    | 35:BA:1253:A:N6     | 2.26                     | 0.50              |
| 35:BA:1503:U:H2'   | 35:BA:1504:C:C5     | 2.46                     | 0.50              |
| 35:BA:1784:A:H4'   | 35:BA:1785:A:H5''   | 1.93                     | 0.50              |
| 35:BA:2040:C:H2'   | 35:BA:2041:U:C6     | 2.46                     | 0.50              |
| 35:BA:2397:G:C2'   | 35:BA:2398:U:H5'    | 2.41                     | 0.50              |
| 35:BA:2475:C:H5'   | 35:BA:2476:A:OP2    | 2.11                     | 0.50              |
| 35:BA:298:G:H5'    | 35:BA:299:A:OP1     | 2.11                     | 0.50              |
| 35:BA:491:G:O2'    | 35:BA:492:A:H5'     | 2.11                     | 0.50              |
| 37:BC:218:THR:HG22 | 37:BC:219:MET:SD    | 2.50                     | 0.50              |
| 41:BG:139:LEU:CD2  | 41:BG:139:LEU:H     | 2.25                     | 0.50              |
| 48:BP:38:GLN:HG3   | 48:BP:39:LYS:N      | 2.24                     | 0.50              |
| 49:BQ:65:PHE:N     | 49:BQ:65:PHE:HD1    | 2.08                     | 0.50              |
| 51:BS:58:LEU:HD21  | 51:BS:68:GLN:CB     | 2.41                     | 0.50              |
| 57:BY:42:VAL:CG2   | 57:BY:67:LEU:HD13   | 2.33                     | 0.50              |
| 1:AA:1041:A:H2'    | 1:AA:1042:G:C8      | 2.46                     | 0.50              |
| 1:AA:1120:G:H2'    | 1:AA:1121:U:C6      | 2.47                     | 0.50              |
| 1:AA:1127:G:O2'    | 1:AA:1128:C:H5'     | 2.12                     | 0.50              |
| 1:AA:1306:A:N6     | 1:AA:1331:G:C1'     | 2.73                     | 0.50              |
| 1:AA:1414:U:H2'    | 1:AA:1415:G:C8      | 2.46                     | 0.50              |
| 1:AA:260:G:H2'     | 1:AA:261:U:C6       | 2.47                     | 0.50              |
| 1:AA:346:G:O2'     | 1:AA:347:G:P        | 2.69                     | 0.50              |
| 1:AA:563:A:OP2     | 1:AA:564:C:OP1      | 2.30                     | 0.50              |
| 1:AA:695:A:H2'     | 1:AA:696:A:C8       | 2.46                     | 0.50              |
| 3:AC:6:HIS:ND1     | 3:AC:8:ILE:HB       | 2.26                     | 0.50              |
| 10:AJ:90:LEU:N     | 10:AJ:91:PRO:CD     | 2.56                     | 0.50              |
| 13:AM:116:THR:O    | 13:AM:117:VAL:CB    | 2.60                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:188:C:C4'     | 20:AT:89:ARG:NH1   | 2.75                     | 0.50              |
| 22:AV:43:C:O2      | 22:AV:43:C:C5'     | 2.59                     | 0.50              |
| 24:AY:100:VAL:HG23 | 24:AY:329:ARG:CB   | 2.40                     | 0.50              |
| 24:AY:146:LEU:HD23 | 24:AY:146:LEU:C    | 2.32                     | 0.50              |
| 1:AA:360:A:OP1     | 24:AY:430:ARG:NH2  | 2.45                     | 0.50              |
| 24:AY:457:LEU:O    | 24:AY:457:LEU:HD23 | 2.12                     | 0.50              |
| 24:AY:628:ARG:NH1  | 24:AY:628:ARG:HG2  | 2.24                     | 0.50              |
| 35:BA:1103:A:C5'   | 35:BA:1104:C:OP2   | 2.46                     | 0.50              |
| 35:BA:2206:G:C3'   | 35:BA:2206:G:N3    | 2.72                     | 0.50              |
| 35:BA:272(B):G:H2' | 35:BA:272(C):G:H8  | 1.76                     | 0.50              |
| 35:BA:860:U:HO2'   | 35:BA:861:A:H5'    | 1.74                     | 0.50              |
| 38:BD:45:ASN:CG    | 38:BD:46:GLN:H     | 2.14                     | 0.50              |
| 39:BE:55:ASN:O     | 39:BE:56:PRO:C     | 2.50                     | 0.50              |
| 41:BG:104:GLU:HA   | 41:BG:107:LEU:HB3  | 1.92                     | 0.50              |
| 41:BG:137:GLU:HA   | 41:BG:155:MET:H    | 1.76                     | 0.50              |
| 42:BH:9:ILE:HG22   | 42:BH:10:PRO:N     | 2.25                     | 0.50              |
| 35:BA:252:G:P      | 48:BP:50:ARG:NH1   | 2.78                     | 0.50              |
| 50:BR:4:LEU:C      | 50:BR:6:SER:H      | 2.14                     | 0.50              |
| 1:AA:1118:C:H1'    | 1:AA:1179:A:C4     | 2.47                     | 0.50              |
| 1:AA:1372:U:H2'    | 1:AA:1373:G:H8     | 1.76                     | 0.50              |
| 1:AA:507:C:C6      | 1:AA:508:C:C6      | 2.99                     | 0.50              |
| 1:AA:559:A:O4'     | 1:AA:561:U:H2'     | 2.10                     | 0.50              |
| 1:AA:614:A:H2'     | 1:AA:615:C:H6      | 1.76                     | 0.50              |
| 1:AA:771:G:O6      | 1:AA:772:U:O4      | 2.30                     | 0.50              |
| 2:AB:148:TYR:O     | 2:AB:149:LEU:HD13  | 2.12                     | 0.50              |
| 2:AB:71:VAL:HG11   | 2:AB:170:GLU:HG2   | 1.93                     | 0.50              |
| 3:AC:34:LEU:HG     | 14:AN:25:VAL:HG11  | 1.94                     | 0.50              |
| 3:AC:40:ARG:NH1    | 3:AC:40:ARG:HG3    | 2.27                     | 0.50              |
| 4:AD:12:CYS:SG     | 4:AD:19:LEU:HB2    | 2.52                     | 0.50              |
| 12:AL:18:VAL:CG2   | 12:AL:19:ARG:N     | 2.70                     | 0.50              |
| 13:AM:9:ILE:O      | 13:AM:10:PRO:O     | 2.30                     | 0.50              |
| 13:AM:4:ILE:CG2    | 13:AM:5:ALA:H      | 2.08                     | 0.50              |
| 14:AN:12:ARG:NH1   | 14:AN:14:PRO:HG2   | 2.26                     | 0.50              |
| 24:AY:128:TYR:HD1  | 24:AY:128:TYR:N    | 2.10                     | 0.50              |
| 24:AY:339:SER:O    | 24:AY:351:ARG:HD2  | 2.11                     | 0.50              |
| 26:B1:57:GLU:CG    | 26:B1:58:ILE:H     | 2.18                     | 0.50              |
| 27:B2:45:SER:O     | 27:B2:47:ASN:OD1   | 2.30                     | 0.50              |
| 28:B3:39:ASP:CG    | 28:B3:44:ARG:HH21  | 2.13                     | 0.50              |
| 29:B4:16:CYS:CA    | 29:B4:33:VAL:HG11  | 2.41                     | 0.50              |
| 29:B4:5:ILE:O      | 29:B4:6:HIS:O      | 2.30                     | 0.50              |
| 35:BA:1036:G:C2    | 35:BA:1120:G:C5    | 3.00                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:1087:G:N2    | 35:BA:1103:A:H61  | 2.03                     | 0.50              |
| 35:BA:1054:A:C6    | 35:BA:1106:G:C6   | 3.00                     | 0.50              |
| 35:BA:1411:C:H2'   | 35:BA:1412:A:C8   | 2.47                     | 0.50              |
| 35:BA:1806:C:H2'   | 35:BA:1807:G:C5'  | 2.41                     | 0.50              |
| 35:BA:1890:A:H3'   | 35:BA:1891:G:H5'  | 1.91                     | 0.50              |
| 35:BA:1914:C:H5''  | 35:BA:1915:U:C5   | 2.46                     | 0.50              |
| 35:BA:2182:G:H2'   | 35:BA:2183:C:C6   | 2.46                     | 0.50              |
| 35:BA:2189:U:C3'   | 35:BA:2190:G:H5'' | 2.40                     | 0.50              |
| 36:BB:101:G:H2'    | 36:BB:102:A:O4'   | 2.12                     | 0.50              |
| 36:BB:22:U:H2'     | 36:BB:23:G:C8     | 2.47                     | 0.50              |
| 37:BC:117:THR:CG2  | 37:BC:119:ASP:OD1 | 2.60                     | 0.50              |
| 39:BE:77:ILE:HG22  | 39:BE:78:LEU:HD12 | 1.93                     | 0.50              |
| 41:BG:24:GLY:O     | 41:BG:25:TYR:CB   | 2.58                     | 0.50              |
| 41:BG:5:VAL:HB     | 41:BG:8:LYS:CB    | 2.41                     | 0.50              |
| 41:BG:7:LEU:O      | 41:BG:8:LYS:C     | 2.50                     | 0.50              |
| 42:BH:124:GLU:HG3  | 42:BH:132:ARG:HG3 | 1.93                     | 0.50              |
| 42:BH:30:LYS:CE    | 42:BH:81:GLU:HG3  | 2.17                     | 0.50              |
| 47:BO:53:LYS:O     | 47:BO:56:ASP:HB2  | 2.12                     | 0.50              |
| 48:BP:71:VAL:HG13  | 48:BP:72:PRO:CD   | 2.41                     | 0.50              |
| 48:BP:95:VAL:HA    | 48:BP:99:LEU:HD23 | 1.94                     | 0.50              |
| 54:BV:47:VAL:C     | 54:BV:49:THR:N    | 2.65                     | 0.50              |
| 49:BQ:141:GLN:HE21 | 58:BZ:72:ARG:HA   | 1.77                     | 0.50              |
| 1:AA:1499:A:OP1    | 1:AA:1499:A:H3'   | 2.12                     | 0.50              |
| 1:AA:437:U:O2'     | 1:AA:438:G:H5'    | 2.11                     | 0.50              |
| 2:AB:105:PHE:O     | 2:AB:109:SER:N    | 2.42                     | 0.50              |
| 2:AB:115:LEU:HD22  | 2:AB:153:ARG:NH1  | 2.26                     | 0.50              |
| 2:AB:16:HIS:CD2    | 2:AB:210:SER:OG   | 2.65                     | 0.50              |
| 3:AC:130:VAL:O     | 3:AC:131:ARG:HB2  | 2.11                     | 0.50              |
| 5:AE:40:ARG:HG2    | 5:AE:40:ARG:HH11  | 1.76                     | 0.50              |
| 9:AI:53:VAL:HG13   | 9:AI:95:LYS:CE    | 2.40                     | 0.50              |
| 15:AO:54:ARG:HG2   | 15:AO:58:MET:CE   | 2.41                     | 0.50              |
| 17:AQ:66:SER:O     | 17:AQ:70:ARG:NH1  | 2.45                     | 0.50              |
| 18:AR:32:ARG:CA    | 18:AR:69:THR:HG21 | 2.32                     | 0.50              |
| 19:AS:58:VAL:O     | 19:AS:58:VAL:HG23 | 2.10                     | 0.50              |
| 19:AS:67:VAL:CG1   | 29:B4:52:THR:HG23 | 2.42                     | 0.50              |
| 24:AY:20:HIS:CG    | 24:AY:115:GLU:HB2 | 2.47                     | 0.50              |
| 24:AY:20:HIS:CD2   | 24:AY:21:ILE:N    | 2.80                     | 0.50              |
| 25:B0:52:GLY:O     | 25:B0:60:PHE:CD1  | 2.64                     | 0.50              |
| 27:B2:2:LYS:HA     | 27:B2:5:GLU:HG2   | 1.94                     | 0.50              |
| 28:B3:35:ARG:HD2   | 28:B3:37:LEU:HD21 | 1.93                     | 0.50              |
| 29:B4:14:ILE:O     | 29:B4:15:ILE:O    | 2.30                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:B4:5:ILE:O     | 29:B4:6:HIS:C      | 2.50                     | 0.50              |
| 35:BA:1464:C:H1'  | 35:BA:1528:A:C8    | 2.47                     | 0.50              |
| 35:BA:1274:A:C2   | 35:BA:1645:G:O4'   | 2.65                     | 0.50              |
| 35:BA:1669:A:O3'  | 35:BA:2549:G:H5'   | 2.12                     | 0.50              |
| 35:BA:1902:C:O2'  | 38:BD:244:ARG:HB3  | 2.06                     | 0.50              |
| 35:BA:2401:U:C5   | 35:BA:2402:C:N4    | 2.79                     | 0.50              |
| 35:BA:2524:G:H2'  | 35:BA:2525:G:O4'   | 2.11                     | 0.50              |
| 35:BA:2893:G:H5'  | 35:BA:2894:G:C5'   | 2.32                     | 0.50              |
| 35:BA:654:A:C8    | 35:BA:654(V):A:H4' | 2.47                     | 0.50              |
| 35:BA:958:U:C2'   | 35:BA:959:A:OP2    | 2.60                     | 0.50              |
| 36:BB:16:G:O2'    | 36:BB:17:C:H6      | 1.92                     | 0.50              |
| 36:BB:66:A:O2'    | 36:BB:67:G:O5'     | 2.30                     | 0.50              |
| 37:BC:108:TRP:O   | 37:BC:110:ASP:N    | 2.45                     | 0.50              |
| 39:BE:33:VAL:HG12 | 39:BE:89:ASP:O     | 2.12                     | 0.50              |
| 40:BF:203:GLN:C   | 40:BF:205:ARG:H    | 2.15                     | 0.50              |
| 41:BG:34:LEU:N    | 41:BG:34:LEU:HD12  | 2.26                     | 0.50              |
| 41:BG:38:VAL:HG13 | 41:BG:93:THR:CA    | 2.41                     | 0.50              |
| 42:BH:37:VAL:HG12 | 42:BH:38:SER:N     | 2.27                     | 0.50              |
| 46:BN:57:ALA:O    | 46:BN:58:ASP:C     | 2.48                     | 0.50              |
| 54:BV:82:ARG:HD2  | 54:BV:82:ARG:N     | 2.26                     | 0.50              |
| 1:AA:1399:C:H1'   | 1:AA:1400:C:OP2    | 2.12                     | 0.50              |
| 1:AA:149:A:O2'    | 1:AA:150:C:H5'     | 2.11                     | 0.50              |
| 1:AA:272:C:O2'    | 1:AA:273:A:H5'     | 2.12                     | 0.50              |
| 1:AA:563:A:O5'    | 1:AA:564:C:OP1     | 2.30                     | 0.50              |
| 1:AA:688:G:N1     | 1:AA:700:G:C6      | 2.80                     | 0.50              |
| 1:AA:962:C:C2'    | 1:AA:963:G:O5'     | 2.60                     | 0.50              |
| 2:AB:157:ARG:O    | 2:AB:158:LEU:O     | 2.30                     | 0.50              |
| 3:AC:129:ALA:CB   | 3:AC:133:ALA:HB2   | 2.42                     | 0.50              |
| 3:AC:94:LEU:C     | 3:AC:94:LEU:HD12   | 2.32                     | 0.50              |
| 5:AE:80:ILE:HD12  | 5:AE:138:ALA:CB    | 2.28                     | 0.50              |
| 8:AH:121:ASP:HB2  | 8:AH:125:ARG:NH2   | 2.26                     | 0.50              |
| 27:B2:70:GLN:O    | 27:B2:71:ASN:C     | 2.50                     | 0.50              |
| 29:B4:36:CYS:O    | 29:B4:38:LYS:HE2   | 2.11                     | 0.50              |
| 30:B5:40:LYS:CE   | 30:B5:46:CYS:CB    | 2.80                     | 0.50              |
| 35:BA:443:A:H1'   | 35:BA:1201:C:O4'   | 2.12                     | 0.50              |
| 35:BA:1416:G:O2'  | 35:BA:1417:C:OP2   | 2.30                     | 0.50              |
| 35:BA:1495:A:N3   | 35:BA:1496:A:C2    | 2.80                     | 0.50              |
| 35:BA:1653:G:O4'  | 35:BA:1654:A:OP2   | 2.30                     | 0.50              |
| 35:BA:2009:G:C6   | 35:BA:2010:G:N7    | 2.79                     | 0.50              |
| 35:BA:2035:G:H4'  | 35:BA:2036:C:OP2   | 2.09                     | 0.50              |
| 35:BA:2145:C:C5'  | 35:BA:2146:C:H5    | 2.25                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2320:A:H8    | 35:BA:2321:G:O6    | 1.95                     | 0.50              |
| 35:BA:2401:U:O2'   | 35:BA:2402:C:OP1   | 2.30                     | 0.50              |
| 35:BA:2461:C:H2'   | 35:BA:2462:U:H6    | 1.75                     | 0.50              |
| 35:BA:271(D):G:O2' | 35:BA:271(E):U:H5' | 2.12                     | 0.50              |
| 35:BA:860:U:C2'    | 35:BA:861:A:C5'    | 2.90                     | 0.50              |
| 36:BB:15:A:H1'     | 36:BB:110:G:C5     | 2.47                     | 0.50              |
| 37:BC:191:ARG:O    | 37:BC:194:ILE:HG22 | 2.12                     | 0.50              |
| 38:BD:21:PHE:C     | 38:BD:24:ILE:HG22  | 2.31                     | 0.50              |
| 39:BE:103:ASP:OD2  | 39:BE:201:THR:HA   | 2.11                     | 0.50              |
| 35:BA:2620:C:P     | 39:BE:153:GLY:H    | 2.34                     | 0.50              |
| 41:BG:133:LEU:HD13 | 41:BG:134:GLY:N    | 2.26                     | 0.50              |
| 43:BJ:72:UNK:C     | 43:BJ:74:UNK:N     | 2.75                     | 0.50              |
| 47:BO:115:VAL:HG13 | 47:BO:121:VAL:HG21 | 1.93                     | 0.50              |
| 48:BP:105:LEU:N    | 48:BP:105:LEU:HD12 | 2.26                     | 0.50              |
| 50:BR:53:HIS:HD2   | 50:BR:94:TYR:OH    | 1.95                     | 0.50              |
| 51:BS:13:ARG:CG    | 51:BS:14:VAL:N     | 2.74                     | 0.50              |
| 51:BS:88:ASP:O     | 51:BS:89:ARG:HB3   | 2.11                     | 0.50              |
| 52:BT:11:GLU:N     | 52:BT:11:GLU:OE1   | 2.44                     | 0.50              |
| 53:BU:59:ARG:HH11  | 53:BU:59:ARG:CG    | 2.25                     | 0.50              |
| 53:BU:92:ARG:NH1   | 54:BV:11:GLN:O     | 2.44                     | 0.50              |
| 57:BY:2:ARG:O      | 57:BY:3:VAL:HB     | 2.11                     | 0.50              |
| 58:BZ:60:GLU:O     | 58:BZ:61:LEU:CG    | 2.60                     | 0.50              |
| 1:AA:1047:G:O2'    | 1:AA:1048:G:C5'    | 2.59                     | 0.50              |
| 1:AA:1132:C:O2'    | 1:AA:1133:G:H5'    | 2.12                     | 0.50              |
| 1:AA:311:C:HO2'    | 1:AA:312:C:H5''    | 1.72                     | 0.50              |
| 1:AA:774:G:H2'     | 1:AA:775:G:C8      | 2.40                     | 0.50              |
| 1:AA:833:U:H2'     | 1:AA:834:C:C6      | 2.46                     | 0.50              |
| 2:AB:76:GLN:NE2    | 2:AB:76:GLN:H      | 2.10                     | 0.50              |
| 2:AB:76:GLN:O      | 2:AB:211:ILE:HD12  | 2.11                     | 0.50              |
| 3:AC:12:LEU:O      | 3:AC:16:ARG:O      | 2.30                     | 0.50              |
| 3:AC:35:GLU:OE1    | 3:AC:95:THR:HG23   | 2.12                     | 0.50              |
| 4:AD:194:LEU:HD22  | 4:AD:194:LEU:N     | 2.27                     | 0.50              |
| 7:AG:86:GLN:O      | 7:AG:87:VAL:HG12   | 2.12                     | 0.50              |
| 9:AI:52:ALA:HB3    | 9:AI:95:LYS:HZ2    | 1.77                     | 0.50              |
| 10:AJ:43:ARG:NH1   | 10:AJ:43:ARG:HG3   | 2.23                     | 0.50              |
| 12:AL:27:LEU:CD1   | 12:AL:28:LYS:H     | 2.11                     | 0.50              |
| 19:AS:19:VAL:CG1   | 19:AS:44:MET:HG2   | 2.41                     | 0.50              |
| 27:B2:35:LEU:C     | 27:B2:37:PHE:N     | 2.64                     | 0.50              |
| 29:B4:22:ILE:HG21  | 41:BG:105:LYS:HB3  | 1.93                     | 0.50              |
| 31:B6:15:GLU:C     | 31:B6:17:LYS:H     | 2.13                     | 0.50              |
| 35:BA:1301:A:N7    | 35:BA:1303:G:C8    | 2.80                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1424:G:H2'   | 35:BA:1425:G:C8    | 2.46                     | 0.50              |
| 35:BA:1425:G:O5'   | 35:BA:1425:G:H8    | 1.95                     | 0.50              |
| 35:BA:1890:A:O5'   | 35:BA:1890:A:H8    | 1.95                     | 0.50              |
| 35:BA:2126:A:O2'   | 35:BA:2127:G:OP2   | 2.30                     | 0.50              |
| 35:BA:2173:A:H5'   | 35:BA:2174:C:OP2   | 2.12                     | 0.50              |
| 35:BA:2386:C:H2'   | 35:BA:2387:U:C6    | 2.47                     | 0.50              |
| 35:BA:265:A:C1'    | 35:BA:266:G:O4'    | 2.59                     | 0.50              |
| 35:BA:271(F):C:H2' | 35:BA:271(G):C:C6  | 2.47                     | 0.50              |
| 35:BA:331:A:O2'    | 35:BA:332:A:O5'    | 2.30                     | 0.50              |
| 35:BA:740:U:H2'    | 35:BA:741:G:H8     | 1.75                     | 0.50              |
| 35:BA:74:A:H5''    | 35:BA:75:G:O4'     | 2.12                     | 0.50              |
| 35:BA:956:G:H2'    | 35:BA:957:A:H2'    | 1.93                     | 0.50              |
| 36:BB:73:A:C4      | 36:BB:105:A:C2     | 3.00                     | 0.50              |
| 37:BC:144:GLY:C    | 37:BC:161:ARG:NH2  | 2.65                     | 0.50              |
| 37:BC:57:GLN:HB2   | 37:BC:202:PRO:HG2  | 1.93                     | 0.50              |
| 38:BD:133:LEU:HA   | 38:BD:136:ILE:HD13 | 1.93                     | 0.50              |
| 41:BG:82:LEU:HD22  | 41:BG:88:ILE:CD1   | 2.41                     | 0.50              |
| 46:BN:128:HIS:C    | 46:BN:128:HIS:CD2  | 2.84                     | 0.50              |
| 48:BP:115:LEU:O    | 48:BP:116:GLY:O    | 2.30                     | 0.50              |
| 48:BP:16:ARG:O     | 48:BP:18:ARG:N     | 2.45                     | 0.50              |
| 48:BP:30:THR:CG2   | 48:BP:31:ALA:N     | 2.74                     | 0.50              |
| 48:BP:39:LYS:HD2   | 48:BP:40:SER:N     | 2.27                     | 0.50              |
| 35:BA:833:U:H4'    | 48:BP:51:PHE:C     | 2.32                     | 0.50              |
| 1:AA:1283:G:O2'    | 1:AA:1284:C:OP2    | 2.30                     | 0.49              |
| 2:AB:90:MET:O      | 2:AB:91:PRO:O      | 2.30                     | 0.49              |
| 3:AC:150:LYS:HB3   | 3:AC:201:TYR:HB2   | 1.94                     | 0.49              |
| 4:AD:13:ARG:HD2    | 4:AD:36:ARG:O      | 2.12                     | 0.49              |
| 6:AF:72:VAL:HG13   | 6:AF:73:ASN:N      | 2.26                     | 0.49              |
| 7:AG:102:ARG:HG3   | 7:AG:102:ARG:HH11  | 1.76                     | 0.49              |
| 7:AG:50:ILE:HD13   | 7:AG:58:PRO:HA     | 1.93                     | 0.49              |
| 7:AG:94:ARG:NH1    | 7:AG:94:ARG:HG3    | 2.26                     | 0.49              |
| 20:AT:94:ALA:O     | 20:AT:95:ALA:HB3   | 2.11                     | 0.49              |
| 22:AV:45:U:O2      | 22:AV:45:U:O5'     | 2.30                     | 0.49              |
| 24:AY:488:THR:HG1  | 24:AY:598:ASP:HB3  | 1.77                     | 0.49              |
| 24:AY:490:PRO:HG3  | 24:AY:515:GLU:HB2  | 1.94                     | 0.49              |
| 25:B0:36:ILE:HD11  | 35:BA:2355:C:H4'   | 1.94                     | 0.49              |
| 31:B6:11:LEU:CD1   | 31:B6:11:LEU:N     | 2.75                     | 0.49              |
| 31:B6:32:ASN:O     | 31:B6:33:LYS:CG    | 2.58                     | 0.49              |
| 35:BA:1062:G:N2    | 35:BA:1076:C:H42   | 2.09                     | 0.49              |
| 35:BA:1423:G:H2'   | 35:BA:1424:G:H8    | 1.76                     | 0.49              |
| 35:BA:1914:C:H3'   | 35:BA:1915:U:H6    | 1.76                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:1917:U:C2'  | 35:BA:1918:A:H5'   | 2.42                     | 0.49              |
| 35:BA:2554:U:C4   | 35:BA:2555:U:O4    | 2.65                     | 0.49              |
| 35:BA:2593:U:H2'  | 35:BA:2594:C:C6    | 2.46                     | 0.49              |
| 35:BA:773:U:H5'   | 38:BD:47:GLY:HA3   | 1.94                     | 0.49              |
| 35:BA:896:A:O2'   | 58:BZ:176:PRO:HG2  | 2.12                     | 0.49              |
| 37:BC:118:PRO:C   | 37:BC:120:VAL:N    | 2.66                     | 0.49              |
| 37:BC:118:PRO:O   | 37:BC:120:VAL:N    | 2.45                     | 0.49              |
| 35:BA:1799:G:C8   | 38:BD:181:GLU:OE2  | 2.56                     | 0.49              |
| 40:BF:81:PRO:O    | 40:BF:82:ILE:O     | 2.30                     | 0.49              |
| 41:BG:106:LEU:HG  | 41:BG:110:ALA:HB3  | 1.94                     | 0.49              |
| 41:BG:110:ALA:HB1 | 41:BG:142:PRO:HB3  | 1.92                     | 0.49              |
| 41:BG:62:LEU:HD12 | 41:BG:62:LEU:N     | 2.26                     | 0.49              |
| 41:BG:66:GLN:NE2  | 41:BG:94:LEU:CG    | 2.72                     | 0.49              |
| 42:BH:158:HIS:CA  | 42:BH:170:ARG:HD2  | 2.40                     | 0.49              |
| 48:BP:47:ASP:OD2  | 48:BP:49:ARG:N     | 2.45                     | 0.49              |
| 50:BR:50:HIS:CE1  | 50:BR:54:LEU:HD11  | 2.47                     | 0.49              |
| 51:BS:99:LYS:NZ   | 51:BS:99:LYS:CB    | 2.75                     | 0.49              |
| 55:BW:68:ARG:HB3  | 55:BW:110:LYS:H    | 1.77                     | 0.49              |
| 56:BX:28:PHE:CZ   | 56:BX:92:LEU:HD11  | 2.47                     | 0.49              |
| 58:BZ:128:VAL:CG1 | 58:BZ:133:ILE:HD13 | 2.42                     | 0.49              |
| 1:AA:1394:A:C5    | 1:AA:1501:C:H4'    | 2.48                     | 0.49              |
| 1:AA:197:A:O2'    | 1:AA:198:G:O5'     | 2.30                     | 0.49              |
| 1:AA:491:G:O2'    | 1:AA:492:G:C5'     | 2.60                     | 0.49              |
| 1:AA:512:U:H2'    | 1:AA:513:C:H6      | 1.75                     | 0.49              |
| 1:AA:56:U:H2'     | 1:AA:57:G:H8       | 1.75                     | 0.49              |
| 1:AA:940:C:H2'    | 1:AA:941:G:H8      | 1.78                     | 0.49              |
| 1:AA:961:U:C3'    | 1:AA:961:U:OP1     | 2.59                     | 0.49              |
| 1:AA:962:C:H2'    | 1:AA:963:G:C8      | 2.46                     | 0.49              |
| 2:AB:25:ASN:O     | 2:AB:28:PHE:N      | 2.46                     | 0.49              |
| 4:AD:121:VAL:N    | 4:AD:126:ILE:HD13  | 2.26                     | 0.49              |
| 5:AE:6:PHE:HB3    | 5:AE:34:VAL:HG22   | 1.94                     | 0.49              |
| 9:AI:16:ARG:HB2   | 9:AI:64:THR:HB     | 1.94                     | 0.49              |
| 11:AK:33:THR:HG22 | 11:AK:39:PRO:HA    | 1.94                     | 0.49              |
| 12:AL:93:LEU:HB3  | 12:AL:96:VAL:CG2   | 2.40                     | 0.49              |
| 13:AM:106:ASN:O   | 13:AM:107:ALA:HB3  | 2.12                     | 0.49              |
| 14:AN:44:LEU:HD12 | 14:AN:44:LEU:O     | 2.11                     | 0.49              |
| 18:AR:68:LYS:O    | 18:AR:72:ARG:HG3   | 2.13                     | 0.49              |
| 19:AS:17:GLU:O    | 19:AS:18:LYS:C     | 2.50                     | 0.49              |
| 19:AS:29:ARG:CB   | 19:AS:48:THR:HB    | 2.32                     | 0.49              |
| 21:AU:3:LYS:HD3   | 21:AU:14:TRP:CD1   | 2.47                     | 0.49              |
| 24:AY:128:TYR:CD1 | 24:AY:128:TYR:N    | 2.80                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:AY:348:ARG:HG2  | 24:AY:382:GLU:HG3   | 1.95                     | 0.49              |
| 24:AY:431:LEU:CD1  | 24:AY:465:ARG:HH12  | 2.24                     | 0.49              |
| 25:B0:26:TYR:O     | 25:B0:29:GLN:HG3    | 2.12                     | 0.49              |
| 25:B0:19:LYS:HZ3   | 25:B0:41:ARG:HH22   | 1.45                     | 0.49              |
| 25:B0:56:ASP:C     | 25:B0:58:THR:H      | 2.15                     | 0.49              |
| 26:B1:83:GLU:OE1   | 26:B1:84:GLY:N      | 2.44                     | 0.49              |
| 29:B4:23:GLU:O     | 29:B4:24:THR:O      | 2.30                     | 0.49              |
| 33:B8:4:MET:HE2    | 33:B8:61:LEU:HB3    | 1.95                     | 0.49              |
| 35:BA:1009:A:C4'   | 53:BU:59:ARG:HD3    | 2.42                     | 0.49              |
| 35:BA:1021:A:H61   | 35:BA:1142(A):A:H61 | 1.61                     | 0.49              |
| 35:BA:1228:G:N2    | 35:BA:1229:G:C1'    | 2.70                     | 0.49              |
| 35:BA:1799:G:C3'   | 35:BA:1799:G:P      | 3.00                     | 0.49              |
| 35:BA:2115:G:H2'   | 35:BA:2117:A:H62    | 1.77                     | 0.49              |
| 35:BA:2524:G:H5'   | 35:BA:2524:G:C8     | 2.44                     | 0.49              |
| 35:BA:2810:A:O2'   | 39:BE:61:ARG:NH1    | 2.45                     | 0.49              |
| 35:BA:2842:G:O2'   | 35:BA:2843:G:H5'    | 2.12                     | 0.49              |
| 35:BA:331:A:C2'    | 35:BA:332:A:OP1     | 2.60                     | 0.49              |
| 37:BC:183:PRO:C    | 37:BC:185:LYS:H     | 2.16                     | 0.49              |
| 37:BC:54:ARG:HD2   | 37:BC:55:SER:H      | 1.76                     | 0.49              |
| 38:BD:70:TRP:CZ3   | 38:BD:146:GLU:OE2   | 2.65                     | 0.49              |
| 39:BE:197:ILE:HD11 | 39:BE:199:ARG:CZ    | 2.42                     | 0.49              |
| 40:BF:65:TRP:CZ3   | 40:BF:72:ARG:HB3    | 2.47                     | 0.49              |
| 41:BG:87:PRO:HG2   | 41:BG:88:ILE:N      | 2.22                     | 0.49              |
| 46:BN:15:LEU:HD12  | 46:BN:136:GLU:HG3   | 1.94                     | 0.49              |
| 48:BP:146:VAL:O    | 48:BP:148:LEU:HG    | 2.13                     | 0.49              |
| 49:BQ:21:THR:HG23  | 49:BQ:101:ARG:HB2   | 1.94                     | 0.49              |
| 30:B5:28:PRO:HD2   | 55:BW:35:ILE:HD12   | 1.94                     | 0.49              |
| 49:BQ:140:ALA:O    | 58:BZ:72:ARG:O      | 2.29                     | 0.49              |
| 1:AA:1267:C:O2'    | 1:AA:1268:A:O4'     | 2.29                     | 0.49              |
| 1:AA:199:G:O2'     | 1:AA:200:G:O5'      | 2.30                     | 0.49              |
| 1:AA:200:G:H8      | 1:AA:200:G:O5'      | 1.95                     | 0.49              |
| 1:AA:223:U:H2'     | 1:AA:224:C:C6       | 2.47                     | 0.49              |
| 1:AA:314:C:O2'     | 1:AA:315:A:C5'      | 2.54                     | 0.49              |
| 1:AA:35:G:HO2'     | 1:AA:36:C:H5'       | 1.76                     | 0.49              |
| 1:AA:60:A:O2'      | 1:AA:61:G:OP2       | 2.30                     | 0.49              |
| 1:AA:648:A:H2'     | 1:AA:649:G:C8       | 2.47                     | 0.49              |
| 1:AA:818:G:O2'     | 1:AA:819:A:H5'      | 2.11                     | 0.49              |
| 1:AA:868:C:H2'     | 1:AA:869:G:C5'      | 2.42                     | 0.49              |
| 2:AB:18:GLY:HA2    | 2:AB:41:ILE:HD12    | 1.93                     | 0.49              |
| 7:AG:18:TYR:HB3    | 7:AG:59:LEU:HD12    | 1.93                     | 0.49              |
| 8:AH:29:SER:HB3    | 8:AH:32:LYS:CG      | 2.42                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:95:LYS:C     | 9:AI:98:PRO:HD2    | 2.32                     | 0.49              |
| 11:AK:34:ASP:HB2  | 11:AK:35:PRO:CD    | 2.42                     | 0.49              |
| 17:AQ:9:VAL:HG11  | 17:AQ:84:LEU:HD13  | 1.94                     | 0.49              |
| 1:AA:1318:A:H1'   | 19:AS:37:ARG:HH21  | 1.77                     | 0.49              |
| 22:AV:46:G:H3'    | 22:AV:47:U:H5'     | 1.94                     | 0.49              |
| 24:AY:192:LEU:O   | 24:AY:192:LEU:HD13 | 2.12                     | 0.49              |
| 24:AY:402:ILE:O   | 24:AY:403:GLU:HB3  | 2.11                     | 0.49              |
| 24:AY:72:CYS:SG   | 24:AY:79:ILE:HB    | 2.52                     | 0.49              |
| 35:BA:1049:C:H2'  | 35:BA:1050:A:H8    | 1.77                     | 0.49              |
| 35:BA:1278:A:O2'  | 35:BA:1279:G:H5'   | 2.11                     | 0.49              |
| 35:BA:1301:A:O2'  | 35:BA:1302:A:O5'   | 2.31                     | 0.49              |
| 35:BA:2074:U:H2'  | 35:BA:2075:U:C6    | 2.47                     | 0.49              |
| 35:BA:2095:C:O2'  | 35:BA:2096:U:H5'   | 2.12                     | 0.49              |
| 35:BA:2321:G:H2'  | 35:BA:2321:G:N3    | 2.27                     | 0.49              |
| 35:BA:2361:A:O2'  | 35:BA:2362:G:H5'   | 2.12                     | 0.49              |
| 35:BA:34:C:O5'    | 35:BA:34:C:C6      | 2.63                     | 0.49              |
| 35:BA:466:A:O4'   | 35:BA:683:C:H4'    | 2.12                     | 0.49              |
| 35:BA:491:G:H2'   | 35:BA:492:A:C8     | 2.48                     | 0.49              |
| 35:BA:720:C:H2'   | 35:BA:721:C:H6     | 1.77                     | 0.49              |
| 35:BA:776:G:H4'   | 35:BA:777:A:O5'    | 2.12                     | 0.49              |
| 25:B0:77:ARG:NH2  | 35:BA:857:C:H5'    | 2.26                     | 0.49              |
| 35:BA:967:C:C3'   | 35:BA:968:G:H5'    | 2.33                     | 0.49              |
| 37:BC:94:TYR:O    | 37:BC:95:VAL:O     | 2.30                     | 0.49              |
| 38:BD:26:LYS:HE2  | 38:BD:26:LYS:HA    | 1.93                     | 0.49              |
| 42:BH:53:GLU:HG3  | 42:BH:54:ARG:N     | 2.27                     | 0.49              |
| 42:BH:83:TYR:O    | 42:BH:84:SER:HB3   | 2.12                     | 0.49              |
| 48:BP:96:THR:HG22 | 48:BP:126:VAL:CB   | 2.41                     | 0.49              |
| 55:BW:71:VAL:CG2  | 55:BW:71:VAL:O     | 2.60                     | 0.49              |
| 57:BY:55:TYR:N    | 57:BY:56:PRO:CD    | 2.74                     | 0.49              |
| 57:BY:68:HIS:ND1  | 57:BY:70:SER:HB3   | 2.27                     | 0.49              |
| 36:BB:75:G:H21    | 58:BZ:85:HIS:CE1   | 2.30                     | 0.49              |
| 1:AA:1217:C:H2'   | 1:AA:1218:C:H6     | 1.77                     | 0.49              |
| 1:AA:1330:U:H5'   | 1:AA:1331:G:OP2    | 2.12                     | 0.49              |
| 1:AA:1395:C:C2'   | 1:AA:1396:A:H5'    | 2.43                     | 0.49              |
| 1:AA:399:G:H2'    | 1:AA:400:C:C6      | 2.48                     | 0.49              |
| 1:AA:549:C:C2'    | 1:AA:550:G:O5'     | 2.60                     | 0.49              |
| 1:AA:983:A:O2'    | 1:AA:1050:G:OP2    | 2.31                     | 0.49              |
| 2:AB:212:GLN:CG   | 2:AB:235:SER:HB2   | 2.42                     | 0.49              |
| 9:AI:117:HIS:C    | 9:AI:118:LYS:HG3   | 2.33                     | 0.49              |
| 1:AA:376:G:H5''   | 16:AP:5:ARG:HB2    | 1.94                     | 0.49              |
| 16:AP:60:LEU:HD21 | 16:AP:66:PRO:HG3   | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:14:ASN:HD21  | 24:AY:80:ASN:ND2   | 2.06                     | 0.49              |
| 24:AY:19:ALA:N     | 24:AY:25:LYS:HD3   | 2.26                     | 0.49              |
| 29:B4:17:GLY:N     | 29:B4:33:VAL:HG11  | 2.26                     | 0.49              |
| 31:B6:40:CYS:SG    | 31:B6:45:LYS:HB2   | 2.53                     | 0.49              |
| 33:B8:54:GLU:HG2   | 33:B8:57:ARG:HH21  | 1.77                     | 0.49              |
| 35:BA:1721:G:C6    | 35:BA:1739:U:H5'   | 2.47                     | 0.49              |
| 35:BA:184:C:H2'    | 35:BA:185:U:H6     | 1.77                     | 0.49              |
| 35:BA:1925:C:C3'   | 35:BA:1926:U:C5'   | 2.90                     | 0.49              |
| 35:BA:2203:U:O3'   | 35:BA:2205:C:OP2   | 2.30                     | 0.49              |
| 35:BA:2464:C:O2'   | 35:BA:2465:C:P     | 2.70                     | 0.49              |
| 35:BA:2580:U:C5'   | 39:BE:131:ALA:N    | 2.75                     | 0.49              |
| 35:BA:259:G:C2'    | 35:BA:260:G:C5'    | 2.90                     | 0.49              |
| 38:BD:241:PRO:O    | 38:BD:242:ARG:CB   | 2.58                     | 0.49              |
| 38:BD:3:VAL:CG1    | 38:BD:17:THR:HB    | 2.42                     | 0.49              |
| 39:BE:38:THR:CG2   | 39:BE:40:GLU:OE1   | 2.60                     | 0.49              |
| 40:BF:156:LEU:HD12 | 40:BF:193:VAL:O    | 2.11                     | 0.49              |
| 40:BF:22:ALA:O     | 40:BF:26:ALA:HB2   | 2.12                     | 0.49              |
| 42:BH:3:ARG:HG3    | 42:BH:3:ARG:HH11   | 1.75                     | 0.49              |
| 44:BK:117:UNK:C    | 44:BK:119:UNK:N    | 2.73                     | 0.49              |
| 46:BN:119:ARG:HG3  | 46:BN:119:ARG:NH1  | 2.27                     | 0.49              |
| 46:BN:19:GLU:O     | 46:BN:59:LYS:O     | 2.30                     | 0.49              |
| 46:BN:2:LYS:O      | 46:BN:4:TYR:CE1    | 2.65                     | 0.49              |
| 49:BQ:141:GLN:HG2  | 58:BZ:72:ARG:HD3   | 1.94                     | 0.49              |
| 51:BS:57:LYS:C     | 51:BS:57:LYS:HD2   | 2.33                     | 0.49              |
| 57:BY:44:ILE:CD1   | 57:BY:65:ALA:HB2   | 2.42                     | 0.49              |
| 58:BZ:114:GLY:O    | 58:BZ:146:ILE:HG22 | 2.12                     | 0.49              |
| 1:AA:1118:C:H1'    | 1:AA:1179:A:C5     | 2.47                     | 0.49              |
| 1:AA:1163:C:H2'    | 1:AA:1164:G:C8     | 2.46                     | 0.49              |
| 1:AA:1452:C:H5'    | 1:AA:1457:G:N7     | 2.27                     | 0.49              |
| 1:AA:1504:G:O4'    | 1:AA:1505:G:OP2    | 2.30                     | 0.49              |
| 1:AA:493:G:H2'     | 1:AA:494:U:H5      | 1.76                     | 0.49              |
| 1:AA:838:G:C2'     | 1:AA:839:U:H5''    | 2.40                     | 0.49              |
| 1:AA:946:A:C6      | 1:AA:947:G:O6      | 2.65                     | 0.49              |
| 15:AO:82:ILE:HD11  | 15:AO:87:ILE:C     | 2.33                     | 0.49              |
| 19:AS:16:LEU:O     | 19:AS:19:VAL:HB    | 2.13                     | 0.49              |
| 24:AY:285:ASP:O    | 24:AY:286:ILE:HD12 | 2.13                     | 0.49              |
| 24:AY:510:VAL:CG1  | 24:AY:511:LYS:N    | 2.76                     | 0.49              |
| 27:B2:42:GLY:O     | 27:B2:43:GLN:O     | 2.31                     | 0.49              |
| 29:B4:53:GLU:CD    | 29:B4:54:GLY:H     | 2.13                     | 0.49              |
| 31:B6:33:LYS:HA    | 31:B6:33:LYS:CE    | 2.38                     | 0.49              |
| 35:BA:1067:A:H3'   | 35:BA:1068:G:H5''  | 1.94                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:BA:1142:U:C2'   | 35:BA:1142(A):A:OP1 | 2.61                     | 0.49              |
| 35:BA:1420:U:O4'   | 35:BA:1420:U:OP1    | 2.30                     | 0.49              |
| 35:BA:1819:A:O4'   | 35:BA:1820:U:OP2    | 2.30                     | 0.49              |
| 35:BA:246:C:O5'    | 35:BA:246:C:H6      | 1.94                     | 0.49              |
| 35:BA:2679:A:O2'   | 35:BA:2680:C:H5'    | 2.13                     | 0.49              |
| 35:BA:363(F):A:O2' | 35:BA:364:C:OP2     | 2.28                     | 0.49              |
| 35:BA:643:A:O2'    | 35:BA:644:A:H5'     | 2.12                     | 0.49              |
| 37:BC:3:LYS:O      | 37:BC:3:LYS:HG2     | 2.13                     | 0.49              |
| 40:BF:10:PRO:CA    | 40:BF:127:GLU:HG2   | 2.41                     | 0.49              |
| 41:BG:20:ILE:O     | 41:BG:21:ARG:CB     | 2.59                     | 0.49              |
| 41:BG:77:ILE:CG2   | 41:BG:78:SER:N      | 2.75                     | 0.49              |
| 35:BA:2311:A:C2    | 41:BG:80:PHE:HD2    | 2.29                     | 0.49              |
| 41:BG:66:GLN:NE2   | 41:BG:94:LEU:CD2    | 2.75                     | 0.49              |
| 42:BH:124:GLU:HB2  | 42:BH:132:ARG:CG    | 2.42                     | 0.49              |
| 47:BO:111:PHE:HB3  | 47:BO:114:ILE:HD13  | 1.95                     | 0.49              |
| 52:BT:27:THR:CG2   | 52:BT:28:VAL:H      | 2.03                     | 0.49              |
| 54:BV:37:VAL:O     | 54:BV:37:VAL:HG23   | 2.13                     | 0.49              |
| 58:BZ:19:ARG:C     | 58:BZ:21:ALA:N      | 2.65                     | 0.49              |
| 58:BZ:17:ALA:HA    | 58:BZ:20:ARG:HD3    | 1.95                     | 0.49              |
| 1:AA:1019:C:O2'    | 1:AA:1020:U:H5'     | 2.13                     | 0.49              |
| 1:AA:1161:C:H2'    | 1:AA:1162:C:C6      | 2.47                     | 0.49              |
| 1:AA:1279:A:C2'    | 1:AA:1282:C:N4      | 2.76                     | 0.49              |
| 1:AA:1376:U:H2'    | 1:AA:1377:A:C8      | 2.47                     | 0.49              |
| 1:AA:1385:G:N2     | 1:AA:1386:G:C4      | 2.81                     | 0.49              |
| 1:AA:1503:A:H3'    | 1:AA:1504:G:H5'     | 1.94                     | 0.49              |
| 1:AA:197:A:O2'     | 1:AA:198:G:C8       | 2.65                     | 0.49              |
| 1:AA:519:C:C2'     | 1:AA:520:A:H5'      | 2.43                     | 0.49              |
| 1:AA:26:A:N6       | 1:AA:558:G:H1'      | 2.28                     | 0.49              |
| 1:AA:60:A:O2'      | 1:AA:61:G:O4'       | 2.30                     | 0.49              |
| 1:AA:78:G:N3       | 1:AA:78:G:H2'       | 2.27                     | 0.49              |
| 1:AA:81:U:H2'      | 1:AA:82:U:H5''      | 1.94                     | 0.49              |
| 2:AB:16:HIS:ND1    | 2:AB:210:SER:OG     | 2.45                     | 0.49              |
| 6:AF:69:GLU:CD     | 6:AF:69:GLU:H       | 2.16                     | 0.49              |
| 10:AJ:8:LEU:HD12   | 10:AJ:8:LEU:N       | 2.27                     | 0.49              |
| 11:AK:44:SER:H     | 11:AK:47:VAL:HB     | 1.78                     | 0.49              |
| 12:AL:41:ARG:HG2   | 12:AL:42:THR:N      | 2.23                     | 0.49              |
| 22:AV:19:G:C6      | 35:BA:2169:A:H1'    | 2.48                     | 0.49              |
| 24:AY:688:ILE:HD12 | 24:AY:688:ILE:N     | 2.28                     | 0.49              |
| 27:B2:2:LYS:CE     | 27:B2:52:ASP:OD1    | 2.61                     | 0.49              |
| 30:B5:46:CYS:SG    | 30:B5:48:GLU:HG2    | 2.53                     | 0.49              |
| 33:B8:23:VAL:HG11  | 33:B8:46:ARG:HD3    | 1.94                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:B5:10:LYS:HG3   | 35:BA:1263:U:H1'  | 1.95                     | 0.49              |
| 35:BA:1408:C:H42   | 35:BA:1594:G:H1   | 1.59                     | 0.49              |
| 35:BA:1462:C:H2'   | 35:BA:1463:C:H6   | 1.77                     | 0.49              |
| 35:BA:16:G:C2'     | 35:BA:17:G:C5'    | 2.89                     | 0.49              |
| 35:BA:1819:A:H5''  | 38:BD:158:ALA:CB  | 2.37                     | 0.49              |
| 35:BA:2023:G:H4'   | 35:BA:2617:C:O3'  | 2.13                     | 0.49              |
| 35:BA:2248:C:C2'   | 35:BA:2249:U:H5'  | 2.42                     | 0.49              |
| 35:BA:2298:A:N6    | 35:BA:2318:G:C8   | 2.76                     | 0.49              |
| 35:BA:2403:C:H6    | 35:BA:2403:C:O5'  | 1.95                     | 0.49              |
| 35:BA:2468:G:N2    | 35:BA:2481:G:O2'  | 2.46                     | 0.49              |
| 35:BA:2728:U:H2'   | 35:BA:2729:G:C8   | 2.48                     | 0.49              |
| 35:BA:53:A:O2'     | 35:BA:54:G:H5'    | 2.11                     | 0.49              |
| 38:BD:145:VAL:HG12 | 38:BD:146:GLU:O   | 2.12                     | 0.49              |
| 38:BD:97:TYR:C     | 38:BD:99:ASP:N    | 2.65                     | 0.49              |
| 41:BG:144:ILE:O    | 41:BG:145:THR:C   | 2.51                     | 0.49              |
| 41:BG:164:GLU:OE1  | 41:BG:164:GLU:HA  | 2.11                     | 0.49              |
| 45:BL:85:UNK:O     | 45:BL:86:UNK:O    | 2.31                     | 0.49              |
| 46:BN:116:LEU:O    | 46:BN:119:ARG:HB2 | 2.12                     | 0.49              |
| 46:BN:89:LYS:O     | 46:BN:93:THR:HG22 | 2.12                     | 0.49              |
| 48:BP:50:ARG:O     | 48:BP:52:GLU:CB   | 2.52                     | 0.49              |
| 49:BQ:39:PRO:O     | 49:BQ:40:ALA:HB2  | 2.13                     | 0.49              |
| 51:BS:39:ILE:HD11  | 51:BS:73:LEU:HD21 | 1.94                     | 0.49              |
| 57:BY:13:VAL:CG2   | 57:BY:72:VAL:HB   | 2.43                     | 0.49              |
| 57:BY:46:LYS:H     | 57:BY:62:GLU:CG   | 2.26                     | 0.49              |
| 57:BY:88:LYS:NZ    | 57:BY:93:GLY:CA   | 2.75                     | 0.49              |
| 58:BZ:79:ARG:C     | 58:BZ:81:ARG:N    | 2.65                     | 0.49              |
| 1:AA:1384:C:C4     | 1:AA:1385:G:N7    | 2.81                     | 0.49              |
| 1:AA:404:U:H2'     | 1:AA:405:U:C6     | 2.47                     | 0.49              |
| 1:AA:415:A:H2'     | 1:AA:416:G:C8     | 2.47                     | 0.49              |
| 1:AA:771:G:N1      | 1:AA:772:U:C4     | 2.80                     | 0.49              |
| 1:AA:942:G:N1      | 1:AA:943:U:C4     | 2.81                     | 0.49              |
| 2:AB:145:LEU:HD23  | 2:AB:149:LEU:HD22 | 1.94                     | 0.49              |
| 2:AB:155:LEU:CD2   | 2:AB:159:PRO:HG3  | 2.37                     | 0.49              |
| 3:AC:84:ILE:O      | 3:AC:87:LEU:N     | 2.46                     | 0.49              |
| 14:AN:24:CYS:HB2   | 14:AN:29:ARG:HB3  | 1.95                     | 0.49              |
| 25:B0:27:GLU:HB2   | 25:B0:68:GLU:HA   | 1.94                     | 0.49              |
| 35:BA:1295:C:H2'   | 35:BA:1296:G:C8   | 2.47                     | 0.49              |
| 35:BA:1496:A:C8    | 35:BA:1577:C:O2'  | 2.66                     | 0.49              |
| 35:BA:1821:A:C2    | 35:BA:1822:G:C5   | 3.01                     | 0.49              |
| 35:BA:189:G:H2'    | 35:BA:205:G:N2    | 2.28                     | 0.49              |
| 35:BA:214:G:H1'    | 35:BA:216:A:O2'   | 2.13                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:2309:A:C2    | 35:BA:2310:A:H2   | 2.30                     | 0.49              |
| 35:BA:2309:A:H2    | 35:BA:2310:A:H2   | 1.60                     | 0.49              |
| 35:BA:2362:G:H2'   | 35:BA:2363:C:H5'  | 1.93                     | 0.49              |
| 35:BA:2410:G:H21   | 35:BA:2411:A:H1'  | 1.77                     | 0.49              |
| 35:BA:2478:A:H2'   | 35:BA:2479:G:O4'  | 2.13                     | 0.49              |
| 35:BA:2656:U:N3    | 35:BA:2665:A:H2   | 1.97                     | 0.49              |
| 35:BA:272(D):G:H1  | 35:BA:364:C:H42   | 1.60                     | 0.49              |
| 35:BA:314:A:O2'    | 35:BA:315:G:H5'   | 2.13                     | 0.49              |
| 38:BD:24:ILE:HD12  | 38:BD:25:THR:H    | 1.78                     | 0.49              |
| 39:BE:154:LYS:O    | 39:BE:155:LYS:O   | 2.30                     | 0.49              |
| 39:BE:176:ILE:HB   | 39:BE:181:LEU:HB2 | 1.93                     | 0.49              |
| 39:BE:181:LEU:HD21 | 52:BT:7:ILE:HG22  | 1.93                     | 0.49              |
| 39:BE:44:TYR:O     | 39:BE:45:THR:CB   | 2.59                     | 0.49              |
| 44:BK:93:UNK:O     | 44:BK:94:UNK:C    | 2.60                     | 0.49              |
| 48:BP:27:HIS:CE1   | 54:BV:82:ARG:O    | 2.66                     | 0.49              |
| 50:BR:3:HIS:O      | 50:BR:5:LYS:HD3   | 2.13                     | 0.49              |
| 57:BY:28:LYS:CA    | 57:BY:38:ILE:H    | 2.25                     | 0.49              |
| 1:AA:1294:G:O2'    | 1:AA:1295:G:H5'   | 2.12                     | 0.49              |
| 1:AA:1372:U:C2'    | 1:AA:1373:G:O5'   | 2.61                     | 0.49              |
| 1:AA:1392:G:O5'    | 1:AA:1392:G:H8    | 1.96                     | 0.49              |
| 1:AA:255:G:H1'     | 17:AQ:16:GLN:HE21 | 1.76                     | 0.49              |
| 1:AA:365:U:O2      | 1:AA:365:U:O5'    | 2.30                     | 0.49              |
| 3:AC:53:ALA:HB2    | 3:AC:115:LEU:CD1  | 2.32                     | 0.49              |
| 3:AC:9:GLY:HA2     | 3:AC:12:LEU:HG    | 1.93                     | 0.49              |
| 5:AE:98:THR:HB     | 5:AE:117:ASP:HB3  | 1.94                     | 0.49              |
| 5:AE:82:VAL:HG11   | 5:AE:137:GLU:HB3  | 1.94                     | 0.49              |
| 6:AF:86:ARG:O      | 6:AF:87:ARG:CB    | 2.61                     | 0.49              |
| 7:AG:7:ALA:O       | 7:AG:8:GLU:CB     | 2.60                     | 0.49              |
| 12:AL:115:LYS:O    | 12:AL:117:ARG:N   | 2.42                     | 0.49              |
| 14:AN:29:ARG:HG2   | 14:AN:40:CYS:HB2  | 1.93                     | 0.49              |
| 16:AP:9:PHE:HB2    | 16:AP:16:HIS:O    | 2.12                     | 0.49              |
| 24:AY:403:GLU:HA   | 24:AY:403:GLU:OE1 | 2.13                     | 0.49              |
| 24:AY:517:LEU:HD11 | 24:AY:564:LYS:HB3 | 1.94                     | 0.49              |
| 61:AY:701:GCP:H3B1 | 62:AY:2001:HOH:O  | 2.13                     | 0.49              |
| 29:B4:11:PRO:HA    | 29:B4:24:THR:HB   | 1.93                     | 0.49              |
| 30:B5:57:VAL:HG12  | 30:B5:58:LEU:HD12 | 1.95                     | 0.49              |
| 35:BA:105:C:H2'    | 35:BA:106:C:H6    | 1.76                     | 0.49              |
| 35:BA:1067:A:H2'   | 35:BA:1067:A:N3   | 2.28                     | 0.49              |
| 35:BA:1231:G:H2'   | 35:BA:1232:G:H8   | 1.76                     | 0.49              |
| 35:BA:2104:G:C1'   | 35:BA:2105:C:P    | 2.99                     | 0.49              |
| 35:BA:2128:C:O2'   | 35:BA:2129:C:OP2  | 2.31                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:247:G:O2'    | 35:BA:248:G:O5'    | 2.30                     | 0.49              |
| 35:BA:248:G:C2     | 35:BA:2431:U:H4'   | 2.47                     | 0.49              |
| 35:BA:2695:C:H2'   | 35:BA:2696:U:C6    | 2.48                     | 0.49              |
| 35:BA:2756:U:O4'   | 35:BA:2757:A:O5'   | 2.30                     | 0.49              |
| 35:BA:2756:U:C4'   | 35:BA:2757:A:O5'   | 2.61                     | 0.49              |
| 35:BA:2756:U:O4    | 35:BA:2759:G:O6    | 2.30                     | 0.49              |
| 35:BA:287:C:H2'    | 35:BA:288:C:H6     | 1.78                     | 0.49              |
| 35:BA:995:C:O2     | 46:BN:4:TYR:OH     | 2.23                     | 0.49              |
| 35:BA:996:A:O2'    | 35:BA:997:G:H5'    | 2.13                     | 0.49              |
| 37:BC:133:GLY:C    | 37:BC:135:ARG:N    | 2.65                     | 0.49              |
| 37:BC:115:VAL:HG23 | 37:BC:145:THR:O    | 2.13                     | 0.49              |
| 40:BF:25:PRO:HB3   | 40:BF:119:ARG:CB   | 2.36                     | 0.49              |
| 41:BG:41:GLN:NE2   | 41:BG:60:LEU:HD22  | 2.27                     | 0.49              |
| 48:BP:120:ALA:HB1  | 48:BP:138:LEU:HD12 | 1.95                     | 0.49              |
| 48:BP:31:ALA:C     | 48:BP:33:ARG:N     | 2.65                     | 0.49              |
| 49:BQ:66:ILE:HD12  | 49:BQ:66:ILE:O     | 2.12                     | 0.49              |
| 51:BS:11:LYS:C     | 51:BS:13:ARG:H     | 2.14                     | 0.49              |
| 58:BZ:6:LYS:H      | 58:BZ:6:LYS:CE     | 2.22                     | 0.49              |
| 1:AA:964:A:C6      | 1:AA:965:A:N6      | 2.79                     | 0.49              |
| 3:AC:16:ARG:HH11   | 3:AC:16:ARG:CB     | 2.24                     | 0.49              |
| 5:AE:64:ARG:HG3    | 5:AE:64:ARG:NH1    | 2.28                     | 0.49              |
| 9:AI:128:ARG:H     | 9:AI:128:ARG:HD3   | 1.77                     | 0.49              |
| 16:AP:47:ASP:CG    | 16:AP:47:ASP:O     | 2.51                     | 0.49              |
| 1:AA:190:U:O2      | 20:AT:105:SER:HB2  | 2.13                     | 0.49              |
| 24:AY:356:LEU:HD23 | 24:AY:356:LEU:C    | 2.33                     | 0.49              |
| 24:AY:617:MET:HG3  | 24:AY:643:ILE:HD11 | 1.94                     | 0.49              |
| 35:BA:1227:G:C4    | 35:BA:1228:G:N7    | 2.81                     | 0.49              |
| 35:BA:1269:A:H61   | 35:BA:2011:U:H3    | 1.60                     | 0.49              |
| 35:BA:2836:U:C4    | 35:BA:2883:A:N6    | 2.81                     | 0.49              |
| 35:BA:332:A:O4'    | 35:BA:333:G:OP1    | 2.30                     | 0.49              |
| 35:BA:856:C:O2'    | 35:BA:857:C:O5'    | 2.30                     | 0.49              |
| 38:BD:25:THR:O     | 38:BD:26:LYS:HB3   | 2.13                     | 0.49              |
| 39:BE:70:ALA:O     | 39:BE:71:GLY:C     | 2.51                     | 0.49              |
| 39:BE:82:ARG:O     | 39:BE:83:ASP:HB2   | 2.12                     | 0.49              |
| 40:BF:4:VAL:HG11   | 40:BF:17:ARG:HE    | 1.77                     | 0.49              |
| 40:BF:54:ARG:NH2   | 40:BF:80:ALA:HB2   | 2.28                     | 0.49              |
| 41:BG:77:ILE:O     | 41:BG:78:SER:OG    | 2.27                     | 0.49              |
| 42:BH:6:ARG:HH11   | 42:BH:6:ARG:HG3    | 1.78                     | 0.49              |
| 35:BA:2415:G:H4'   | 48:BP:67:MET:N     | 2.28                     | 0.49              |
| 54:BV:21:ARG:HH11  | 54:BV:21:ARG:HG2   | 1.78                     | 0.49              |
| 1:AA:1049:U:C4'    | 1:AA:1050:G:O5'    | 2.49                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1053:G:O2'    | 1:AA:1054:C:OP2    | 2.29                     | 0.49              |
| 1:AA:1333:A:H2'    | 1:AA:1334:G:O4'    | 2.13                     | 0.49              |
| 1:AA:1366:C:C4     | 1:AA:1367:C:N4     | 2.81                     | 0.49              |
| 1:AA:1523:G:O2'    | 1:AA:1524:C:H5'    | 2.12                     | 0.49              |
| 1:AA:184:G:H2'     | 1:AA:185:A:H8      | 1.78                     | 0.49              |
| 1:AA:594:G:H2'     | 1:AA:595:G:C5'     | 2.42                     | 0.49              |
| 1:AA:861:G:H8      | 1:AA:861:G:O5'     | 1.95                     | 0.49              |
| 2:AB:166:ASP:CG    | 2:AB:169:LYS:HB2   | 2.33                     | 0.49              |
| 4:AD:158:ILE:CG2   | 4:AD:181:MET:HE2   | 2.42                     | 0.49              |
| 9:AI:26:VAL:HG22   | 9:AI:27:THR:H      | 1.78                     | 0.49              |
| 13:AM:10:PRO:CG    | 13:AM:18:ALA:HB1   | 2.40                     | 0.49              |
| 19:AS:41:VAL:HG21  | 19:AS:44:MET:HG3   | 1.94                     | 0.49              |
| 20:AT:26:ASN:HD22  | 20:AT:26:ASN:N     | 2.11                     | 0.49              |
| 21:AU:2:GLY:O      | 21:AU:4:GLY:N      | 2.46                     | 0.49              |
| 24:AY:120:THR:HG23 | 24:AY:123:ARG:HH22 | 1.77                     | 0.49              |
| 24:AY:308:PRO:HB2  | 24:AY:394:ALA:CB   | 2.41                     | 0.49              |
| 24:AY:422:GLU:O    | 24:AY:426:GLN:HB2  | 2.13                     | 0.49              |
| 24:AY:47:GLU:HB3   | 24:AY:52:MET:CB    | 2.42                     | 0.49              |
| 24:AY:55:MET:SD    | 24:AY:65:ILE:HD11  | 2.53                     | 0.49              |
| 29:B4:65:ASP:O     | 29:B4:66:SER:C     | 2.51                     | 0.49              |
| 30:B5:41:PRO:HG2   | 30:B5:44:THR:CG2   | 2.39                     | 0.49              |
| 34:B9:10:ILE:N     | 34:B9:10:ILE:HD12  | 2.28                     | 0.49              |
| 35:BA:1062:G:OP2   | 35:BA:1062:G:H8    | 1.96                     | 0.49              |
| 35:BA:1121:C:C2'   | 35:BA:1122:G:O5'   | 2.61                     | 0.49              |
| 35:BA:1181:C:C2'   | 35:BA:1182:A:H5'   | 2.43                     | 0.49              |
| 35:BA:1297:C:C2'   | 35:BA:1298:C:H5'   | 2.41                     | 0.49              |
| 35:BA:1427:A:C1'   | 35:BA:1428:C:OP2   | 2.61                     | 0.49              |
| 35:BA:1453:U:OP1   | 50:BR:77:ARG:NH1   | 2.45                     | 0.49              |
| 35:BA:1887:C:C3'   | 35:BA:1888:G:H5''  | 2.43                     | 0.49              |
| 35:BA:18:C:C2      | 35:BA:19:C:C6      | 3.00                     | 0.49              |
| 35:BA:18:C:N3      | 35:BA:19:C:C4      | 2.81                     | 0.49              |
| 35:BA:2404:C:N4    | 35:BA:2414:G:N1    | 2.61                     | 0.49              |
| 35:BA:2068:U:N3    | 35:BA:2430:A:C2    | 2.56                     | 0.49              |
| 35:BA:953:A:C6     | 35:BA:965:C:N3     | 2.81                     | 0.49              |
| 39:BE:129:HIS:O    | 39:BE:130:GLY:O    | 2.31                     | 0.49              |
| 42:BH:6:ARG:HG3    | 42:BH:6:ARG:NH1    | 2.27                     | 0.49              |
| 45:BL:86:UNK:C     | 45:BL:88:UNK:N     | 2.71                     | 0.49              |
| 46:BN:25:ARG:HH11  | 46:BN:25:ARG:CG    | 2.24                     | 0.49              |
| 47:BO:104:ARG:HB2  | 47:BO:104:ARG:NH1  | 2.27                     | 0.49              |
| 52:BT:106:SER:CA   | 52:BT:110:ILE:HG12 | 2.38                     | 0.49              |
| 54:BV:19:LYS:HE2   | 54:BV:20:LEU:H     | 1.78                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:BY:41:GLY:O     | 57:BY:42:VAL:C     | 2.50                     | 0.49              |
| 1:AA:105:G:H2'     | 1:AA:106:C:C5      | 2.47                     | 0.48              |
| 1:AA:1177:G:H8     | 1:AA:1177:G:O5'    | 1.96                     | 0.48              |
| 1:AA:1367:C:C2'    | 1:AA:1368:G:O5'    | 2.61                     | 0.48              |
| 1:AA:1447:A:H3'    | 1:AA:1447:A:N3     | 2.27                     | 0.48              |
| 1:AA:362:G:H8      | 1:AA:362:G:O5'     | 1.94                     | 0.48              |
| 1:AA:495:A:C4'     | 1:AA:496:A:OP1     | 2.61                     | 0.48              |
| 2:AB:122:PHE:HE2   | 2:AB:139:LYS:HA    | 1.75                     | 0.48              |
| 3:AC:155:GLY:HA3   | 3:AC:196:LEU:HD13  | 1.94                     | 0.48              |
| 3:AC:38:ARG:HB2    | 3:AC:38:ARG:HH11   | 1.78                     | 0.48              |
| 4:AD:31:CYS:SG     | 4:AD:31:CYS:O      | 2.71                     | 0.48              |
| 6:AF:89:MET:HG2    | 6:AF:91:VAL:HG23   | 1.95                     | 0.48              |
| 24:AY:32:ILE:HG23  | 24:AY:273:LEU:HD21 | 1.95                     | 0.48              |
| 24:AY:99:ARG:CD    | 24:AY:402:ILE:H    | 2.26                     | 0.48              |
| 25:B0:50:ASN:CB    | 25:B0:63:VAL:HG21  | 2.43                     | 0.48              |
| 29:B4:10:VAL:HG23  | 29:B4:11:PRO:HD2   | 1.94                     | 0.48              |
| 29:B4:21:VAL:CG2   | 29:B4:35:VAL:HG21  | 2.43                     | 0.48              |
| 29:B4:6:HIS:O      | 29:B4:7:PRO:O      | 2.30                     | 0.48              |
| 34:B9:1:MET:SD     | 34:B9:31:LYS:C     | 2.92                     | 0.48              |
| 35:BA:1426:G:OP2   | 35:BA:1427:A:O2'   | 2.30                     | 0.48              |
| 35:BA:1504:C:O2'   | 35:BA:1505:C:C5'   | 2.60                     | 0.48              |
| 35:BA:1899:G:O2'   | 35:BA:1900:A:H5''  | 2.12                     | 0.48              |
| 35:BA:1985:G:C2'   | 35:BA:1986:A:O5'   | 2.60                     | 0.48              |
| 35:BA:2123:G:H2'   | 35:BA:2124:G:H5'   | 1.92                     | 0.48              |
| 35:BA:2199:A:H2'   | 35:BA:2199:A:N3    | 2.27                     | 0.48              |
| 35:BA:2757:A:O2'   | 35:BA:2758:A:C5'   | 2.57                     | 0.48              |
| 35:BA:436:C:H2'    | 35:BA:437:G:H8     | 1.78                     | 0.48              |
| 35:BA:464:U:H6     | 35:BA:464:U:O5'    | 1.96                     | 0.48              |
| 35:BA:18:C:O2'     | 35:BA:554:U:OP1    | 2.31                     | 0.48              |
| 35:BA:652:C:O2'    | 35:BA:653:A:O5'    | 2.31                     | 0.48              |
| 35:BA:680:G:H2'    | 35:BA:681:G:C8     | 2.48                     | 0.48              |
| 35:BA:690:G:H2'    | 35:BA:691:C:C6     | 2.48                     | 0.48              |
| 35:BA:782:A:H5'    | 35:BA:783:A:C2     | 2.48                     | 0.48              |
| 35:BA:858:U:O2'    | 35:BA:859:G:C8     | 2.56                     | 0.48              |
| 35:BA:958:U:H6     | 35:BA:958:U:H3'    | 1.78                     | 0.48              |
| 37:BC:184:GLU:O    | 37:BC:188:ASP:OD2  | 2.31                     | 0.48              |
| 41:BG:127:GLY:C    | 41:BG:129:GLY:N    | 2.65                     | 0.48              |
| 41:BG:133:LEU:CD1  | 41:BG:134:GLY:H    | 2.24                     | 0.48              |
| 41:BG:162:THR:HG22 | 41:BG:163:ALA:N    | 2.28                     | 0.48              |
| 41:BG:80:PHE:O     | 41:BG:81:LYS:CG    | 2.61                     | 0.48              |
| 54:BV:14:VAL:HB    | 54:BV:96:ILE:HG13  | 1.94                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 56:BX:36:LYS:HD3   | 56:BX:54:VAL:O    | 2.13                     | 0.48              |
| 57:BY:50:ARG:HD2   | 57:BY:54:LYS:O    | 2.13                     | 0.48              |
| 58:BZ:115:GLY:HA2  | 58:BZ:177:PRO:CD  | 2.41                     | 0.48              |
| 1:AA:1030(D):A:O2' | 1:AA:1031:G:P     | 2.70                     | 0.48              |
| 1:AA:1153:C:O2'    | 1:AA:1154:G:O5'   | 2.30                     | 0.48              |
| 1:AA:335:C:H2'     | 1:AA:336:C:H6     | 1.78                     | 0.48              |
| 1:AA:34:C:O2'      | 1:AA:35:G:H5'     | 2.13                     | 0.48              |
| 1:AA:442:C:H42     | 1:AA:492:G:H1     | 1.62                     | 0.48              |
| 1:AA:980:C:H2'     | 1:AA:981:U:H5'    | 1.94                     | 0.48              |
| 2:AB:82:ARG:HG2    | 2:AB:83:MET:N     | 2.26                     | 0.48              |
| 3:AC:40:ARG:HG3    | 3:AC:40:ARG:HH11  | 1.78                     | 0.48              |
| 3:AC:84:ILE:HG23   | 3:AC:85:ARG:H     | 1.77                     | 0.48              |
| 4:AD:36:ARG:HH11   | 4:AD:36:ARG:HB3   | 1.78                     | 0.48              |
| 1:AA:667:G:H4'     | 15:AO:51:HIS:ND1  | 2.27                     | 0.48              |
| 19:AS:17:GLU:O     | 19:AS:19:VAL:N    | 2.46                     | 0.48              |
| 31:B6:20:ASN:CG    | 31:B6:21:TYR:N    | 2.67                     | 0.48              |
| 33:B8:24:ALA:O     | 33:B8:46:ARG:HA   | 2.12                     | 0.48              |
| 35:BA:1144:G:C6    | 35:BA:1145:C:N4   | 2.81                     | 0.48              |
| 35:BA:1296:G:C2'   | 35:BA:1297:C:H5'  | 2.43                     | 0.48              |
| 35:BA:1416:G:N2    | 35:BA:1417:C:C2   | 2.82                     | 0.48              |
| 35:BA:1579:A:H2'   | 35:BA:1580:A:O4'  | 2.14                     | 0.48              |
| 35:BA:1415:U:H3    | 35:BA:1587:A:H61  | 1.62                     | 0.48              |
| 35:BA:1595:G:H2'   | 35:BA:1596:A:H5'  | 1.95                     | 0.48              |
| 35:BA:1645:G:O5'   | 35:BA:1645:G:H8   | 1.96                     | 0.48              |
| 35:BA:17:G:C4      | 35:BA:18:C:C5     | 3.00                     | 0.48              |
| 35:BA:1848:A:H3'   | 35:BA:1848:A:OP1  | 2.13                     | 0.48              |
| 35:BA:1925:C:O2    | 35:BA:1925:C:H2'  | 2.12                     | 0.48              |
| 35:BA:1992:G:O4'   | 35:BA:1993:U:OP2  | 2.30                     | 0.48              |
| 35:BA:2009:G:O2'   | 35:BA:2010:G:H5'' | 2.13                     | 0.48              |
| 35:BA:2103:C:O2'   | 35:BA:2104:G:C5'  | 2.59                     | 0.48              |
| 35:BA:2169:A:O2'   | 35:BA:2170:A:H5'  | 2.13                     | 0.48              |
| 35:BA:2103:C:N4    | 35:BA:2186:G:H1   | 2.08                     | 0.48              |
| 35:BA:2197:U:O2'   | 35:BA:2198:A:H2'  | 2.13                     | 0.48              |
| 35:BA:2606:C:O5'   | 35:BA:2606:C:H6   | 1.96                     | 0.48              |
| 35:BA:2651:C:O2'   | 35:BA:2652:C:H5'  | 2.12                     | 0.48              |
| 35:BA:2770:G:H5'   | 35:BA:2771:C:OP2  | 2.13                     | 0.48              |
| 35:BA:2807:G:C2'   | 35:BA:2808:U:H5'' | 2.42                     | 0.48              |
| 35:BA:29:U:H2'     | 35:BA:30:G:H5'    | 1.88                     | 0.48              |
| 35:BA:605:C:H1'    | 35:BA:657:U:HO2'  | 1.78                     | 0.48              |
| 35:BA:869:G:O2'    | 35:BA:870:A:H5'   | 2.13                     | 0.48              |
| 38:BD:21:PHE:O     | 38:BD:24:ILE:HG22 | 2.13                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:BD:89:SER:HB2   | 38:BD:159:ALA:H   | 1.78                     | 0.48              |
| 40:BF:46:ARG:HG3   | 40:BF:46:ARG:NH1  | 2.29                     | 0.48              |
| 41:BG:118:ARG:HD3  | 41:BG:118:ARG:H   | 1.78                     | 0.48              |
| 41:BG:40:ASN:HD21  | 41:BG:91:ARG:HG3  | 1.77                     | 0.48              |
| 46:BN:45:ASN:HD22  | 46:BN:45:ASN:H    | 1.58                     | 0.48              |
| 48:BP:65:ARG:HB3   | 48:BP:68:GLN:NE2  | 2.08                     | 0.48              |
| 25:B0:7:LEU:HD12   | 49:BQ:85:LYS:HE2  | 1.93                     | 0.48              |
| 54:BV:2:PHE:HD1    | 54:BV:3:ALA:N     | 2.11                     | 0.48              |
| 35:BA:143:G:H4'    | 56:BX:35:THR:HG21 | 1.95                     | 0.48              |
| 1:AA:1385:G:C2'    | 1:AA:1386:G:O5'   | 2.61                     | 0.48              |
| 1:AA:265:G:H2'     | 1:AA:267:C:C5     | 2.48                     | 0.48              |
| 1:AA:486:U:H2'     | 1:AA:487:A:C8     | 2.48                     | 0.48              |
| 1:AA:723:U:C2'     | 1:AA:723:U:O2     | 2.61                     | 0.48              |
| 1:AA:773:G:N1      | 1:AA:774:G:C6     | 2.81                     | 0.48              |
| 1:AA:863:U:O2      | 1:AA:863:U:H5'    | 2.13                     | 0.48              |
| 2:AB:130:ARG:HE    | 2:AB:131:PRO:HD2  | 1.79                     | 0.48              |
| 3:AC:11:ARG:O      | 3:AC:14:ILE:N     | 2.38                     | 0.48              |
| 4:AD:13:ARG:HG2    | 4:AD:33:MET:HE3   | 1.94                     | 0.48              |
| 4:AD:159:ARG:HH11  | 4:AD:159:ARG:HB3  | 1.78                     | 0.48              |
| 11:AK:15:ALA:HA    | 11:AK:76:GLY:O    | 2.13                     | 0.48              |
| 20:AT:26:ASN:ND2   | 20:AT:26:ASN:N    | 2.60                     | 0.48              |
| 22:AV:63:G:H2'     | 22:AV:64:A:O4'    | 2.14                     | 0.48              |
| 24:AY:47:GLU:HB3   | 24:AY:52:MET:HA   | 1.94                     | 0.48              |
| 24:AY:606:MET:HE3  | 24:AY:671:MET:HG3 | 1.96                     | 0.48              |
| 24:AY:623:ASP:O    | 24:AY:626:ALA:HB3 | 2.13                     | 0.48              |
| 24:AY:628:ARG:HH11 | 24:AY:628:ARG:CG  | 2.16                     | 0.48              |
| 24:AY:680:PRO:HD2  | 24:AY:683:VAL:CG2 | 2.40                     | 0.48              |
| 25:B0:53:MET:SD    | 25:B0:57:PHE:CA   | 3.00                     | 0.48              |
| 27:B2:69:ARG:O     | 27:B2:70:GLN:OE1  | 2.31                     | 0.48              |
| 28:B3:36:VAL:O     | 28:B3:36:VAL:HG23 | 2.12                     | 0.48              |
| 29:B4:47:GLN:O     | 29:B4:48:ARG:C    | 2.51                     | 0.48              |
| 30:B5:3:LYS:HG3    | 30:B5:4:HIS:H     | 1.77                     | 0.48              |
| 30:B5:53:ALA:O     | 30:B5:55:ARG:N    | 2.46                     | 0.48              |
| 31:B6:42:TRP:HA    | 31:B6:42:TRP:HE3  | 1.77                     | 0.48              |
| 31:B6:53:LYS:HD3   | 31:B6:54:ILE:N    | 2.22                     | 0.48              |
| 35:BA:1684:C:H2'   | 35:BA:1685:C:H6   | 1.77                     | 0.48              |
| 35:BA:1967:C:N4    | 35:BA:1968:G:C6   | 2.81                     | 0.48              |
| 35:BA:1968:G:O2'   | 35:BA:1969:A:O4'  | 2.30                     | 0.48              |
| 35:BA:2033:A:O2'   | 35:BA:2034:U:O5'  | 2.30                     | 0.48              |
| 35:BA:2142:C:O2'   | 35:BA:2143:C:H5'  | 2.13                     | 0.48              |
| 35:BA:2559:C:H2'   | 35:BA:2560:C:H5'  | 1.94                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:271(P):C:C2' | 35:BA:271(Q):G:H5' | 2.43                     | 0.48              |
| 35:BA:39:C:H2'     | 35:BA:40:C:C6      | 2.48                     | 0.48              |
| 35:BA:621:A:H2'    | 35:BA:622:G:C5'    | 2.42                     | 0.48              |
| 35:BA:738:G:O6     | 35:BA:739:G:N1     | 2.46                     | 0.48              |
| 35:BA:848:G:N9     | 35:BA:933:A:H8     | 2.12                     | 0.48              |
| 35:BA:890:A:H2'    | 35:BA:892:G:H5''   | 1.94                     | 0.48              |
| 37:BC:81:GLY:O     | 37:BC:82:GLU:HB3   | 2.12                     | 0.48              |
| 38:BD:117:VAL:HG22 | 38:BD:118:VAL:N    | 2.28                     | 0.48              |
| 38:BD:97:TYR:C     | 38:BD:99:ASP:H     | 2.17                     | 0.48              |
| 40:BF:19:GLU:CD    | 40:BF:19:GLU:N     | 2.67                     | 0.48              |
| 41:BG:55:LYS:HB3   | 41:BG:148:MET:HE1  | 1.96                     | 0.48              |
| 48:BP:9:ASN:N      | 48:BP:10:PRO:HD2   | 2.27                     | 0.48              |
| 35:BA:2485:G:H5''  | 49:BQ:46:GLN:HE21  | 1.78                     | 0.48              |
| 52:BT:38:ASN:HD22  | 52:BT:38:ASN:H     | 1.61                     | 0.48              |
| 57:BY:39:VAL:O     | 57:BY:40:GLU:CG    | 2.60                     | 0.48              |
| 36:BB:77:U:P       | 58:BZ:19:ARG:NH2   | 2.86                     | 0.48              |
| 1:AA:1239:A:H62    | 1:AA:1299:A:H61    | 1.60                     | 0.48              |
| 1:AA:490:G:H2'     | 1:AA:491:G:C5'     | 2.43                     | 0.48              |
| 4:AD:149:ALA:O     | 4:AD:153:ARG:HG3   | 2.13                     | 0.48              |
| 7:AG:49:ILE:HD11   | 7:AG:118:VAL:HA    | 1.94                     | 0.48              |
| 9:AI:50:LEU:HD23   | 9:AI:85:LEU:CD2    | 2.44                     | 0.48              |
| 9:AI:92:TYR:O      | 9:AI:95:LYS:HG3    | 2.14                     | 0.48              |
| 13:AM:96:LEU:HB3   | 13:AM:97:PRO:CD    | 2.41                     | 0.48              |
| 24:AY:315:LYS:HB3  | 24:AY:327:PHE:HD2  | 1.78                     | 0.48              |
| 29:B4:29:PRO:HG2   | 29:B4:30:GLU:H     | 1.78                     | 0.48              |
| 29:B4:56:VAL:C     | 29:B4:58:ARG:H     | 2.16                     | 0.48              |
| 35:BA:528:A:C2     | 35:BA:2043:C:C5'   | 2.96                     | 0.48              |
| 35:BA:2151:G:OP1   | 37:BC:3:LYS:HE2    | 2.12                     | 0.48              |
| 35:BA:2481:G:O2'   | 35:BA:2482:G:OP2   | 2.30                     | 0.48              |
| 35:BA:36:G:C6      | 35:BA:37:C:C4      | 3.02                     | 0.48              |
| 35:BA:34:C:H42     | 35:BA:447:A:H61    | 1.61                     | 0.48              |
| 37:BC:101:ILE:C    | 37:BC:103:LYS:N    | 2.67                     | 0.48              |
| 37:BC:129:GLY:O    | 37:BC:133:GLY:N    | 2.29                     | 0.48              |
| 39:BE:68:ALA:C     | 39:BE:70:ALA:N     | 2.66                     | 0.48              |
| 40:BF:133:ASN:HD22 | 40:BF:133:ASN:N    | 2.10                     | 0.48              |
| 40:BF:89:VAL:CG1   | 40:BF:90:PHE:N     | 2.63                     | 0.48              |
| 48:BP:85:LEU:HD22  | 48:BP:115:LEU:O    | 2.13                     | 0.48              |
| 53:BU:42:ALA:O     | 53:BU:43:GLY:C     | 2.51                     | 0.48              |
| 54:BV:15:GLU:CG    | 54:BV:16:PRO:CD    | 2.86                     | 0.48              |
| 54:BV:72:VAL:HG23  | 54:BV:72:VAL:O     | 2.13                     | 0.48              |
| 57:BY:28:LYS:HB2   | 57:BY:37:VAL:CB    | 2.22                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:BY:3:VAL:C      | 57:BY:5:MET:H      | 2.15                     | 0.48              |
| 57:BY:95:LYS:CE    | 57:BY:99:CYS:O     | 2.61                     | 0.48              |
| 57:BY:81:LYS:CD    | 57:BY:97:ARG:HG3   | 2.38                     | 0.48              |
| 1:AA:454:C:H5'     | 1:AA:455:C:OP2     | 2.13                     | 0.48              |
| 1:AA:484:G:H4'     | 1:AA:485:G:O5'     | 2.14                     | 0.48              |
| 1:AA:519:C:H2'     | 1:AA:520:A:H5'     | 1.95                     | 0.48              |
| 1:AA:697:U:O2'     | 1:AA:698:G:H5'     | 2.13                     | 0.48              |
| 2:AB:132:LYS:HG3   | 2:AB:135:GLN:OE1   | 2.13                     | 0.48              |
| 4:AD:104:VAL:O     | 4:AD:108:LEU:HB2   | 2.13                     | 0.48              |
| 7:AG:131:LYS:N     | 7:AG:131:LYS:HD2   | 2.29                     | 0.48              |
| 12:AL:18:VAL:O     | 12:AL:19:ARG:HB3   | 2.13                     | 0.48              |
| 13:AM:112:GLY:HA3  | 13:AM:115:LYS:HE2  | 1.93                     | 0.48              |
| 20:AT:23:ARG:HH11  | 20:AT:23:ARG:HG2   | 1.79                     | 0.48              |
| 24:AY:127:LYS:C    | 24:AY:128:TYR:HD1  | 2.16                     | 0.48              |
| 24:AY:401:SER:O    | 24:AY:402:ILE:CB   | 2.61                     | 0.48              |
| 24:AY:44:GLU:C     | 24:AY:45:VAL:HG13  | 2.33                     | 0.48              |
| 24:AY:538:TYR:CD1  | 24:AY:579:GLU:HG2  | 2.48                     | 0.48              |
| 24:AY:138:LYS:HG2  | 61:AY:701:GCP:C4   | 2.43                     | 0.48              |
| 24:AY:99:ARG:HD2   | 24:AY:402:ILE:H    | 1.78                     | 0.48              |
| 25:B0:19:LYS:HG3   | 25:B0:41:ARG:HH21  | 1.79                     | 0.48              |
| 25:B0:49:LYS:O     | 25:B0:50:ASN:HB2   | 2.14                     | 0.48              |
| 28:B3:5:LYS:CE     | 28:B3:34:GLU:OE2   | 2.61                     | 0.48              |
| 29:B4:2:LYS:HD3    | 29:B4:2:LYS:O      | 2.13                     | 0.48              |
| 29:B4:60:GLN:C     | 29:B4:62:ARG:HD2   | 2.33                     | 0.48              |
| 29:B4:9:LEU:HD12   | 29:B4:9:LEU:N      | 2.28                     | 0.48              |
| 33:B8:32:LEU:HB2   | 33:B8:36:LYS:HZ1   | 1.75                     | 0.48              |
| 33:B8:4:MET:HG2    | 33:B8:61:LEU:CD2   | 2.43                     | 0.48              |
| 35:BA:1188:U:H4'   | 54:BV:79:VAL:HG13  | 1.95                     | 0.48              |
| 35:BA:570:G:H2'    | 35:BA:2030:A:C5    | 2.49                     | 0.48              |
| 35:BA:2287:A:N6    | 35:BA:2344:U:N3    | 2.57                     | 0.48              |
| 35:BA:2410:G:C2    | 35:BA:2411:A:C4    | 3.01                     | 0.48              |
| 35:BA:2457:U:O2'   | 35:BA:2458:G:H5'   | 2.13                     | 0.48              |
| 35:BA:332:A:C6     | 35:BA:335:C:C4     | 3.01                     | 0.48              |
| 35:BA:331:A:O4'    | 35:BA:332:A:OP1    | 2.32                     | 0.48              |
| 33:B8:15:LYS:HE3   | 35:BA:630:G:OP2    | 2.14                     | 0.48              |
| 35:BA:872:A:H4'    | 49:BQ:66:ILE:HD11  | 1.94                     | 0.48              |
| 37:BC:88:GLU:O     | 37:BC:89:GLU:HB3   | 2.14                     | 0.48              |
| 38:BD:133:LEU:HB3  | 38:BD:173:VAL:HG11 | 1.94                     | 0.48              |
| 38:BD:260:ARG:HH22 | 38:BD:266:SER:HB3  | 1.79                     | 0.48              |
| 43:BJ:70:UNK:O     | 43:BJ:71:UNK:CB    | 2.61                     | 0.48              |
| 46:BN:30:ILE:HG22  | 46:BN:34:LEU:HD22  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BN:22:THR:CG2  | 46:BN:61:ARG:HD3   | 2.40                     | 0.48              |
| 46:BN:67:LEU:O    | 46:BN:68:GLU:CB    | 2.61                     | 0.48              |
| 49:BQ:52:VAL:HA   | 49:BQ:55:VAL:CG1   | 2.44                     | 0.48              |
| 51:BS:89:ARG:HG3  | 51:BS:92:TYR:CA    | 2.43                     | 0.48              |
| 53:BU:110:VAL:O   | 53:BU:114:LYS:HG2  | 2.13                     | 0.48              |
| 55:BW:59:VAL:O    | 55:BW:63:ASP:HA    | 2.13                     | 0.48              |
| 58:BZ:121:HIS:HB2 | 58:BZ:171:ILE:HA   | 1.95                     | 0.48              |
| 1:AA:1123:A:O2'   | 10:AJ:38:ILE:HG22  | 2.14                     | 0.48              |
| 1:AA:1152:A:C2    | 1:AA:1153:C:C4     | 3.01                     | 0.48              |
| 1:AA:123:C:H2'    | 1:AA:124:G:H8      | 1.79                     | 0.48              |
| 1:AA:60:A:O2'     | 1:AA:61:G:O5'      | 2.32                     | 0.48              |
| 1:AA:853:G:O2'    | 1:AA:854:G:H5'     | 2.13                     | 0.48              |
| 1:AA:995:C:H4'    | 14:AN:8:GLU:OE2    | 2.14                     | 0.48              |
| 2:AB:141:GLU:O    | 2:AB:144:ARG:HG2   | 2.13                     | 0.48              |
| 2:AB:87:ARG:HD2   | 2:AB:219:VAL:CG1   | 2.27                     | 0.48              |
| 3:AC:28:GLN:O     | 3:AC:31:HIS:N      | 2.47                     | 0.48              |
| 6:AF:44:GLY:HA2   | 6:AF:59:TYR:CE1    | 2.49                     | 0.48              |
| 7:AG:47:CYS:CA    | 7:AG:50:ILE:HG22   | 2.42                     | 0.48              |
| 9:AI:10:ARG:O     | 9:AI:11:LYS:C      | 2.52                     | 0.48              |
| 10:AJ:23:ILE:HG23 | 10:AJ:85:LEU:HD22  | 1.95                     | 0.48              |
| 12:AL:53:ARG:HH12 | 12:AL:92:ASP:HB2   | 1.79                     | 0.48              |
| 19:AS:32:LYS:HA   | 19:AS:50:ALA:HB3   | 1.95                     | 0.48              |
| 19:AS:41:VAL:CB   | 19:AS:44:MET:HB3   | 2.37                     | 0.48              |
| 20:AT:26:ASN:H    | 20:AT:26:ASN:ND2   | 2.11                     | 0.48              |
| 24:AY:34:TYR:O    | 24:AY:38:ARG:HB2   | 2.12                     | 0.48              |
| 24:AY:421:GLN:C   | 24:AY:421:GLN:HE21 | 2.17                     | 0.48              |
| 25:B0:19:LYS:HE2  | 25:B0:19:LYS:HA    | 1.95                     | 0.48              |
| 27:B2:5:GLU:O     | 27:B2:8:LYS:HG3    | 2.14                     | 0.48              |
| 31:B6:26:ASN:HD21 | 31:B6:32:ASN:HD22  | 1.60                     | 0.48              |
| 35:BA:1090:U:H2'  | 35:BA:1091:G:C8    | 2.49                     | 0.48              |
| 35:BA:1140:C:H6   | 35:BA:1140:C:O5'   | 1.97                     | 0.48              |
| 35:BA:1319:G:O2'  | 35:BA:1320:C:H5'   | 2.13                     | 0.48              |
| 35:BA:1458:C:H4'  | 35:BA:1459:G:C4    | 2.49                     | 0.48              |
| 35:BA:1771:C:H1'  | 35:BA:1786:A:C8    | 2.48                     | 0.48              |
| 35:BA:2011:U:C2'  | 35:BA:2012:G:O5'   | 2.61                     | 0.48              |
| 35:BA:2175:C:C2   | 35:BA:2176:A:N7    | 2.82                     | 0.48              |
| 35:BA:2383:G:O2'  | 35:BA:2384:G:H5'   | 2.13                     | 0.48              |
| 35:BA:256:A:C2'   | 35:BA:257:A:C5'    | 2.80                     | 0.48              |
| 35:BA:2692:C:H1'  | 35:BA:2847:U:O2'   | 2.13                     | 0.48              |
| 35:BA:2713:A:O2'  | 35:BA:2714:G:H5''  | 2.14                     | 0.48              |
| 35:BA:607:U:N3    | 35:BA:620:G:C8     | 2.82                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:635:C:O2'    | 35:BA:639:U:OP1    | 2.31                     | 0.48              |
| 35:BA:780:G:H21    | 35:BA:783:A:H62    | 1.60                     | 0.48              |
| 36:BB:17:C:H2'     | 36:BB:18:G:O4'     | 2.14                     | 0.48              |
| 36:BB:55:U:H2'     | 36:BB:56:G:C8      | 2.48                     | 0.48              |
| 38:BD:147:LEU:HD22 | 38:BD:155:LEU:HD11 | 1.94                     | 0.48              |
| 38:BD:28:GLU:CD    | 38:BD:28:GLU:N     | 2.66                     | 0.48              |
| 38:BD:33:LEU:C     | 38:BD:33:LEU:HD23  | 2.34                     | 0.48              |
| 39:BE:132:HIS:CG   | 39:BE:132:HIS:O    | 2.64                     | 0.48              |
| 41:BG:106:LEU:HA   | 41:BG:110:ALA:HB2  | 1.96                     | 0.48              |
| 35:BA:2305:A:H5''  | 41:BG:134:GLY:HA3  | 1.95                     | 0.48              |
| 29:B4:28:LYS:CD    | 41:BG:143:GLU:HA   | 2.38                     | 0.48              |
| 48:BP:30:THR:HG22  | 48:BP:31:ALA:H     | 1.75                     | 0.48              |
| 35:BA:2820:A:H1'   | 50:BR:5:LYS:HE3    | 1.95                     | 0.48              |
| 51:BS:102:ALA:O    | 51:BS:103:GLU:HG2  | 2.13                     | 0.48              |
| 51:BS:30:ARG:NH1   | 51:BS:97:ARG:HB3   | 2.28                     | 0.48              |
| 52:BT:117:ASP:O    | 52:BT:119:LYS:N    | 2.46                     | 0.48              |
| 52:BT:23:ARG:CB    | 52:BT:24:PRO:HD2   | 2.23                     | 0.48              |
| 53:BU:92:ARG:NH1   | 53:BU:94:ASN:ND2   | 2.57                     | 0.48              |
| 1:AA:390:C:H2'     | 1:AA:391:G:C8      | 2.49                     | 0.48              |
| 1:AA:405:U:O2      | 1:AA:498:U:H2'     | 2.14                     | 0.48              |
| 1:AA:567:G:H2'     | 1:AA:568:G:O4'     | 2.14                     | 0.48              |
| 1:AA:590:C:C2'     | 1:AA:591:U:C5'     | 2.90                     | 0.48              |
| 1:AA:961:U:HO2'    | 1:AA:962:C:H6      | 1.62                     | 0.48              |
| 2:AB:111:ARG:HG3   | 2:AB:145:LEU:HD21  | 1.94                     | 0.48              |
| 3:AC:22:TRP:HB2    | 3:AC:59:ARG:HB2    | 1.96                     | 0.48              |
| 12:AL:94:PRO:C     | 12:AL:96:VAL:H     | 2.17                     | 0.48              |
| 17:AQ:95:TYR:C     | 17:AQ:97:SER:H     | 2.17                     | 0.48              |
| 24:AY:99:ARG:NH2   | 24:AY:128:TYR:OH   | 2.46                     | 0.48              |
| 25:B0:42:GLY:O     | 25:B0:57:PHE:CB    | 2.62                     | 0.48              |
| 32:B7:23:ARG:NH1   | 32:B7:23:ARG:HG3   | 2.28                     | 0.48              |
| 35:BA:1062:G:H22   | 35:BA:1076:C:H42   | 1.61                     | 0.48              |
| 35:BA:140:G:N3     | 35:BA:142:A:N1     | 2.61                     | 0.48              |
| 35:BA:146:G:H2'    | 35:BA:147:U:O4'    | 2.14                     | 0.48              |
| 35:BA:1820:U:C4    | 38:BD:160:GLY:O    | 2.65                     | 0.48              |
| 35:BA:1982:C:N3    | 35:BA:1983:C:N4    | 2.60                     | 0.48              |
| 35:BA:246:C:C3'    | 35:BA:247:G:C5'    | 2.91                     | 0.48              |
| 35:BA:248:G:C8     | 35:BA:250:G:C4     | 3.02                     | 0.48              |
| 35:BA:271(M):G:N7  | 35:BA:271(O):C:C4  | 2.82                     | 0.48              |
| 35:BA:333:G:C6     | 35:BA:334:C:N4     | 2.82                     | 0.48              |
| 35:BA:35:G:H2'     | 35:BA:36:G:C8      | 2.48                     | 0.48              |
| 35:BA:387:U:H6     | 35:BA:387:U:O5'    | 1.96                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:435:C:H2'   | 35:BA:436:C:H5'    | 1.95                     | 0.48              |
| 35:BA:48:G:C6     | 35:BA:178:G:O6     | 2.66                     | 0.48              |
| 35:BA:534:U:H5'   | 53:BU:42:ALA:HB1   | 1.96                     | 0.48              |
| 35:BA:644:A:H2'   | 35:BA:646:A:C2     | 2.49                     | 0.48              |
| 35:BA:743:G:O2'   | 35:BA:744:G:O5'    | 2.30                     | 0.48              |
| 35:BA:856:C:C4'   | 35:BA:857:C:OP1    | 2.57                     | 0.48              |
| 35:BA:968:G:C2'   | 35:BA:969:U:C5'    | 2.92                     | 0.48              |
| 37:BC:42:VAL:HA   | 37:BC:216:THR:O    | 2.13                     | 0.48              |
| 39:BE:141:ILE:HB  | 39:BE:154:LYS:HE2  | 1.95                     | 0.48              |
| 39:BE:56:PRO:O    | 39:BE:57:LYS:NZ    | 2.47                     | 0.48              |
| 40:BF:133:ASN:O   | 40:BF:134:GLY:C    | 2.52                     | 0.48              |
| 42:BH:16:SER:HB2  | 42:BH:27:LYS:HB2   | 1.94                     | 0.48              |
| 35:BA:558:G:P     | 46:BN:111:PRO:HD2  | 2.53                     | 0.48              |
| 47:BO:17:ARG:HE   | 47:BO:47:ILE:HD12  | 1.78                     | 0.48              |
| 48:BP:24:GLY:N    | 48:BP:33:ARG:CZ    | 2.76                     | 0.48              |
| 48:BP:51:PHE:CD2  | 48:BP:52:GLU:C     | 2.87                     | 0.48              |
| 49:BQ:50:ALA:O    | 49:BQ:53:ALA:HB3   | 2.14                     | 0.48              |
| 50:BR:103:ARG:NH1 | 50:BR:110:PRO:HB3  | 2.28                     | 0.48              |
| 35:BA:1249:U:O4'  | 53:BU:4:ALA:HB3    | 2.14                     | 0.48              |
| 54:BV:21:ARG:HG3  | 54:BV:93:GLU:HB2   | 1.96                     | 0.48              |
| 54:BV:61:VAL:HG12 | 54:BV:94:LEU:CD2   | 2.43                     | 0.48              |
| 57:BY:38:ILE:HG22 | 57:BY:39:VAL:N     | 2.27                     | 0.48              |
| 35:BA:896:A:C8    | 58:BZ:146:ILE:HD12 | 2.49                     | 0.48              |
| 58:BZ:72:ARG:HG2  | 58:BZ:89:PHE:HB2   | 1.96                     | 0.48              |
| 1:AA:1151:A:H1'   | 1:AA:1152:A:C8     | 2.48                     | 0.48              |
| 1:AA:1305:G:O2'   | 1:AA:1306:A:O5'    | 2.30                     | 0.48              |
| 1:AA:1401:G:H2'   | 1:AA:1402:C:O4'    | 2.13                     | 0.48              |
| 1:AA:193:C:H2'    | 1:AA:194:C:C6      | 2.48                     | 0.48              |
| 1:AA:339:C:OP2    | 47:BO:97:ARG:NH1   | 2.46                     | 0.48              |
| 1:AA:339:C:H2'    | 1:AA:340:U:C6      | 2.48                     | 0.48              |
| 1:AA:453:A:O2'    | 1:AA:454:C:O4'     | 2.32                     | 0.48              |
| 1:AA:591:U:H2'    | 1:AA:592:G:H8      | 1.79                     | 0.48              |
| 2:AB:74:LYS:O     | 2:AB:74:LYS:HG3    | 2.14                     | 0.48              |
| 3:AC:167:TRP:CD1  | 3:AC:168:ALA:N     | 2.82                     | 0.48              |
| 5:AE:100:VAL:O    | 5:AE:100:VAL:HG23  | 2.13                     | 0.48              |
| 7:AG:22:LEU:O     | 7:AG:24:THR:N      | 2.38                     | 0.48              |
| 10:AJ:32:ALA:HB2  | 10:AJ:81:THR:HG21  | 1.95                     | 0.48              |
| 19:AS:42:PRO:HB3  | 19:AS:67:VAL:HG13  | 1.95                     | 0.48              |
| 20:AT:36:LEU:HD13 | 20:AT:55:ILE:HG23  | 1.95                     | 0.48              |
| 24:AY:272:LEU:O   | 24:AY:276:VAL:HG23 | 2.13                     | 0.48              |
| 24:AY:497:PHE:CE2 | 24:AY:581:ALA:HA   | 2.49                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:B1:39:LYS:NZ    | 35:BA:189:G:OP2    | 2.47                     | 0.48              |
| 31:B6:15:GLU:OE1   | 31:B6:18:ARG:CG    | 2.61                     | 0.48              |
| 31:B6:26:ASN:ND2   | 31:B6:32:ASN:ND2   | 2.61                     | 0.48              |
| 31:B6:53:LYS:CD    | 31:B6:54:ILE:N     | 2.76                     | 0.48              |
| 33:B8:4:MET:O      | 33:B8:62:LEU:HD11  | 2.14                     | 0.48              |
| 33:B8:61:LEU:HD13  | 33:B8:62:LEU:H     | 1.78                     | 0.48              |
| 35:BA:1215:G:O6    | 35:BA:1235:G:N3    | 2.47                     | 0.48              |
| 35:BA:1430:C:H2'   | 35:BA:1431:U:C6    | 2.48                     | 0.48              |
| 35:BA:1786:A:N3    | 35:BA:1786:A:H2'   | 2.29                     | 0.48              |
| 35:BA:19:C:O2'     | 35:BA:20:C:H5'     | 2.13                     | 0.48              |
| 30:B5:51:TYR:OH    | 35:BA:2884:U:C2    | 2.55                     | 0.48              |
| 35:BA:971:C:OP1    | 35:BA:974:G:C8     | 2.67                     | 0.48              |
| 36:BB:65:C:O2'     | 36:BB:66:A:H5'     | 2.13                     | 0.48              |
| 36:BB:80:U:H2'     | 36:BB:81:G:N2      | 2.22                     | 0.48              |
| 37:BC:125:GLY:O    | 37:BC:127:LYS:HG2  | 2.13                     | 0.48              |
| 38:BD:142:VAL:CG2  | 38:BD:191:ALA:HB1  | 2.43                     | 0.48              |
| 38:BD:36:PRO:O     | 38:BD:37:LEU:HG    | 2.14                     | 0.48              |
| 39:BE:120:TRP:CE3  | 39:BE:155:LYS:HE2  | 2.48                     | 0.48              |
| 39:BE:188:VAL:O    | 39:BE:188:VAL:HG13 | 2.14                     | 0.48              |
| 39:BE:60:ASN:OD1   | 39:BE:62:PRO:CD    | 2.53                     | 0.48              |
| 41:BG:6:ALA:CB     | 41:BG:105:LYS:HZ2  | 2.22                     | 0.48              |
| 55:BW:73:ALA:HB3   | 55:BW:106:ILE:HG12 | 1.95                     | 0.48              |
| 56:BX:35:THR:HG22  | 56:BX:36:LYS:N     | 2.27                     | 0.48              |
| 58:BZ:155:LEU:CD2  | 58:BZ:155:LEU:H    | 2.27                     | 0.48              |
| 1:AA:1154:G:N3     | 1:AA:1155:G:C8     | 2.82                     | 0.48              |
| 1:AA:1370:G:C2     | 1:AA:1371:G:N7     | 2.82                     | 0.48              |
| 1:AA:1387:G:C2'    | 1:AA:1388:C:H5'    | 2.42                     | 0.48              |
| 1:AA:484:G:H8      | 1:AA:484:G:OP1     | 1.96                     | 0.48              |
| 1:AA:667:G:H4'     | 15:AO:51:HIS:CE1   | 2.48                     | 0.48              |
| 1:AA:770:C:HO2'    | 1:AA:771:G:H5'     | 1.66                     | 0.48              |
| 1:AA:89:C:C2       | 1:AA:90:U:C5       | 3.02                     | 0.48              |
| 4:AD:36:ARG:CB     | 4:AD:36:ARG:HH11   | 2.26                     | 0.48              |
| 7:AG:15:ASP:OD2    | 7:AG:23:VAL:HG11   | 2.13                     | 0.48              |
| 11:AK:69:ALA:O     | 11:AK:72:ALA:N     | 2.47                     | 0.48              |
| 13:AM:65:LYS:HB2   | 13:AM:69:GLU:CG    | 2.43                     | 0.48              |
| 24:AY:148:LEU:O    | 24:AY:152:THR:HG22 | 2.14                     | 0.48              |
| 24:AY:196:ILE:HG13 | 24:AY:197:ARG:N    | 2.21                     | 0.48              |
| 24:AY:249:GLY:C    | 24:AY:255:ILE:HG23 | 2.34                     | 0.48              |
| 24:AY:25:LYS:HZ3   | 24:AY:86:GLY:HA3   | 1.79                     | 0.48              |
| 24:AY:384:ILE:HG12 | 24:AY:387:ASP:OD2  | 2.13                     | 0.48              |
| 24:AY:438:PHE:CE1  | 24:AY:451:ILE:HG13 | 2.48                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:B3:59:VAL:CG1   | 28:B3:60:GLU:N    | 2.75                     | 0.48              |
| 31:B6:35:GLU:HB3   | 31:B6:51:GLU:HG3  | 1.96                     | 0.48              |
| 31:B6:35:GLU:HB3   | 31:B6:51:GLU:CG   | 2.44                     | 0.48              |
| 35:BA:1099:G:O2'   | 35:BA:1100:C:H5'  | 2.14                     | 0.48              |
| 35:BA:1169:G:H2'   | 35:BA:1170:G:O4'  | 2.14                     | 0.48              |
| 35:BA:1295:C:H2'   | 35:BA:1296:G:H8   | 1.78                     | 0.48              |
| 35:BA:1683:C:H2'   | 35:BA:1684:C:C6   | 2.49                     | 0.48              |
| 35:BA:1893:C:H2'   | 35:BA:1894:C:C5'  | 2.43                     | 0.48              |
| 35:BA:2126:A:C6    | 35:BA:2163:C:H4'  | 2.48                     | 0.48              |
| 25:B0:12:ASN:HB2   | 35:BA:2278:A:C8   | 2.49                     | 0.48              |
| 35:BA:250:G:H2'    | 35:BA:251:A:C8    | 2.49                     | 0.48              |
| 35:BA:271(D):G:H2' | 35:BA:271(E):U:H6 | 1.78                     | 0.48              |
| 35:BA:848:G:C4     | 35:BA:933:A:H8    | 2.31                     | 0.48              |
| 22:AV:55:U:OP2     | 37:BC:142:LYS:HD2 | 2.14                     | 0.48              |
| 38:BD:263:ARG:HB2  | 38:BD:263:ARG:CZ  | 2.44                     | 0.48              |
| 40:BF:185:ASP:HA   | 40:BF:188:ARG:HD3 | 1.95                     | 0.48              |
| 40:BF:20:LEU:HB3   | 40:BF:23:ASP:OD1  | 2.14                     | 0.48              |
| 36:BB:50:G:OP2     | 51:BS:62:LYS:HB2  | 2.14                     | 0.48              |
| 51:BS:73:LEU:HD23  | 51:BS:73:LEU:C    | 2.34                     | 0.48              |
| 52:BT:35:LYS:NZ    | 52:BT:41:ARG:HE   | 2.12                     | 0.48              |
| 53:BU:92:ARG:CB    | 54:BV:11:GLN:NE2  | 2.76                     | 0.48              |
| 1:AA:1152:A:N1     | 1:AA:1153:C:N4    | 2.62                     | 0.48              |
| 1:AA:1371:G:HO2'   | 1:AA:1372:U:H5'   | 1.78                     | 0.48              |
| 1:AA:161:A:H2'     | 1:AA:162:A:C8     | 2.49                     | 0.48              |
| 1:AA:452:A:O2'     | 1:AA:453:A:H5'    | 2.14                     | 0.48              |
| 1:AA:509:A:OP2     | 1:AA:510:A:OP2    | 2.32                     | 0.48              |
| 1:AA:521:G:O2'     | 1:AA:522:C:C5'    | 2.59                     | 0.48              |
| 2:AB:114:ARG:NH1   | 2:AB:118:LEU:CD1  | 2.72                     | 0.48              |
| 2:AB:142:LEU:O     | 2:AB:146:GLN:HB2  | 2.14                     | 0.48              |
| 2:AB:16:HIS:CG     | 2:AB:210:SER:OG   | 2.66                     | 0.48              |
| 2:AB:17:PHE:CD1    | 2:AB:18:GLY:N     | 2.81                     | 0.48              |
| 6:AF:69:GLU:CD     | 6:AF:69:GLU:N     | 2.68                     | 0.48              |
| 7:AG:26:PHE:HD1    | 7:AG:101:LEU:HD22 | 1.79                     | 0.48              |
| 16:AP:70:ALA:O     | 16:AP:74:LEU:HG   | 2.13                     | 0.48              |
| 19:AS:19:VAL:HG13  | 19:AS:44:MET:HG2  | 1.96                     | 0.48              |
| 29:B4:1:MET:O      | 29:B4:2:LYS:CB    | 2.58                     | 0.48              |
| 34:B9:18:ARG:HG2   | 34:B9:18:ARG:HH11 | 1.79                     | 0.48              |
| 35:BA:1465:G:C4    | 35:BA:1466:G:C8   | 3.02                     | 0.48              |
| 35:BA:177:G:OP2    | 35:BA:177:G:N2    | 2.41                     | 0.48              |
| 35:BA:2257:U:O2'   | 35:BA:2258:C:H5'  | 2.14                     | 0.48              |
| 35:BA:425:G:O2'    | 35:BA:426:C:H5'   | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BA:654(A):G:N1 | 35:BA:654(S):G:N2 | 2.61                     | 0.48              |
| 35:BA:743:G:C6    | 35:BA:755:C:N3    | 2.81                     | 0.48              |
| 35:BA:99:U:C4'    | 35:BA:102:G:H1'   | 2.44                     | 0.48              |
| 37:BC:158:LYS:O   | 37:BC:159:ALA:CB  | 2.62                     | 0.48              |
| 37:BC:88:GLU:CA   | 37:BC:92:ALA:HB3  | 2.43                     | 0.48              |
| 38:BD:23:GLU:O    | 38:BD:24:ILE:O    | 2.32                     | 0.48              |
| 38:BD:30:GLU:CG   | 38:BD:63:ARG:HE   | 2.26                     | 0.48              |
| 38:BD:95:LEU:HD13 | 38:BD:97:TYR:CE1  | 2.49                     | 0.48              |
| 40:BF:54:ARG:HB2  | 40:BF:79:GLY:O    | 2.13                     | 0.48              |
| 40:BF:9:ILE:O     | 40:BF:11:VAL:N    | 2.47                     | 0.48              |
| 47:BO:66:LYS:HA   | 47:BO:79:PHE:O    | 2.13                     | 0.48              |
| 53:BU:16:LYS:O    | 53:BU:20:LEU:HD22 | 2.14                     | 0.48              |
| 53:BU:88:ILE:O    | 53:BU:88:ILE:HG13 | 2.14                     | 0.48              |
| 54:BV:19:LYS:HZ1  | 54:BV:20:LEU:H    | 1.61                     | 0.48              |
| 54:BV:47:VAL:HG12 | 54:BV:52:VAL:N    | 2.29                     | 0.48              |
| 57:BY:13:VAL:HG22 | 57:BY:14:LEU:N    | 2.29                     | 0.48              |
| 58:BZ:19:ARG:C    | 58:BZ:21:ALA:H    | 2.16                     | 0.48              |
| 1:AA:1015:A:H1'   | 1:AA:1218:C:O2'   | 2.14                     | 0.47              |
| 1:AA:1153:C:O2'   | 1:AA:1154:G:OP2   | 2.30                     | 0.47              |
| 1:AA:1504:G:H3'   | 1:AA:1504:G:OP2   | 2.14                     | 0.47              |
| 1:AA:187:C:O5'    | 1:AA:187:C:H6     | 1.97                     | 0.47              |
| 1:AA:560:U:O2'    | 1:AA:561:U:OP2    | 2.30                     | 0.47              |
| 1:AA:952:U:H2'    | 1:AA:953:G:H5'    | 1.96                     | 0.47              |
| 2:AB:23:ARG:CG    | 2:AB:23:ARG:NH1   | 2.37                     | 0.47              |
| 3:AC:23:TYR:CG    | 3:AC:24:ALA:N     | 2.82                     | 0.47              |
| 4:AD:36:ARG:O     | 4:AD:38:TYR:N     | 2.46                     | 0.47              |
| 1:AA:624:C:H4'    | 16:AP:10:GLY:O    | 2.14                     | 0.47              |
| 16:AP:27:LYS:HG2  | 16:AP:30:GLY:H    | 1.79                     | 0.47              |
| 16:AP:53:VAL:HG12 | 16:AP:79:VAL:HG22 | 1.96                     | 0.47              |
| 1:AA:247:G:OP2    | 17:AQ:99:SER:HB2  | 2.13                     | 0.47              |
| 19:AS:18:LYS:O    | 19:AS:22:LEU:HB2  | 2.14                     | 0.47              |
| 24:AY:229:LEU:C   | 24:AY:231:TYR:N   | 2.66                     | 0.47              |
| 35:BA:1239:G:H2'  | 35:BA:1240:U:O4'  | 2.14                     | 0.47              |
| 35:BA:1786:A:C2'  | 35:BA:1786:A:N3   | 2.77                     | 0.47              |
| 35:BA:18:C:N3     | 35:BA:19:C:C5     | 2.81                     | 0.47              |
| 35:BA:2104:G:N3   | 35:BA:2104:G:H2'  | 2.29                     | 0.47              |
| 35:BA:2206:G:C2'  | 35:BA:2206:G:N3   | 2.76                     | 0.47              |
| 35:BA:2746:U:C2'  | 35:BA:2747:G:H5'  | 2.44                     | 0.47              |
| 35:BA:2807:G:H2'  | 35:BA:2808:U:H5'' | 1.96                     | 0.47              |
| 35:BA:326:G:H2'   | 35:BA:327:G:H8    | 1.78                     | 0.47              |
| 35:BA:47:C:N4     | 35:BA:179:G:H1    | 2.12                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:583:G:OP2    | 53:BU:10:ARG:HD2  | 2.14                     | 0.47              |
| 35:BA:627:A:O2'    | 35:BA:636:G:N2    | 2.47                     | 0.47              |
| 35:BA:859:G:N2     | 35:BA:917:A:OP2   | 2.36                     | 0.47              |
| 35:BA:963:U:H2'    | 35:BA:964:C:O5'   | 2.14                     | 0.47              |
| 38:BD:35:LYS:CD    | 38:BD:35:LYS:C    | 2.82                     | 0.47              |
| 41:BG:49:ASP:O     | 41:BG:50:ALA:C    | 2.52                     | 0.47              |
| 41:BG:80:PHE:O     | 41:BG:81:LYS:HG2  | 2.14                     | 0.47              |
| 42:BH:86:GLU:OE1   | 42:BH:86:GLU:N    | 2.47                     | 0.47              |
| 44:BK:15:UNK:HA    | 44:BK:45:UNK:O    | 2.13                     | 0.47              |
| 46:BN:128:HIS:HD2  | 46:BN:130:HIS:N   | 2.08                     | 0.47              |
| 54:BV:71:LEU:HD12  | 54:BV:86:GLY:HA2  | 1.95                     | 0.47              |
| 55:BW:32:ALA:O     | 55:BW:36:LEU:HD22 | 2.14                     | 0.47              |
| 57:BY:47:LYS:HG3   | 57:BY:60:PHE:CZ   | 2.49                     | 0.47              |
| 1:AA:1239:A:O2'    | 1:AA:1240:U:OP2   | 2.28                     | 0.47              |
| 1:AA:1305:G:OP2    | 1:AA:1305:G:H8    | 1.97                     | 0.47              |
| 1:AA:1396:A:C4'    | 1:AA:1398:A:H1'   | 2.44                     | 0.47              |
| 1:AA:521:G:H2'     | 1:AA:522:C:C5'    | 2.25                     | 0.47              |
| 1:AA:778:G:O2'     | 1:AA:779:C:H5'    | 2.14                     | 0.47              |
| 1:AA:868:C:HO2'    | 1:AA:869:G:H5'    | 1.74                     | 0.47              |
| 13:AM:54:VAL:HA    | 13:AM:57:ARG:HB3  | 1.96                     | 0.47              |
| 15:AO:72:ARG:HG2   | 15:AO:73:GLU:OE2  | 2.14                     | 0.47              |
| 22:AV:45:U:O2      | 22:AV:45:U:C4'    | 2.62                     | 0.47              |
| 24:AY:550:MET:HG2  | 24:AY:560:VAL:HB  | 1.97                     | 0.47              |
| 28:B3:46:ASN:ND2   | 35:BA:850:C:O2'   | 2.47                     | 0.47              |
| 29:B4:31:ILE:HG12  | 29:B4:33:VAL:N    | 2.29                     | 0.47              |
| 35:BA:1215:G:O6    | 35:BA:1235:G:C2   | 2.67                     | 0.47              |
| 26:B1:3:LYS:NZ     | 35:BA:1364:G:N7   | 2.46                     | 0.47              |
| 35:BA:1448:G:H1'   | 35:BA:1528:A:N6   | 2.26                     | 0.47              |
| 35:BA:1698:A:N3    | 35:BA:1700:A:O4'  | 2.47                     | 0.47              |
| 35:BA:2207:G:HO2'  | 35:BA:2208:A:H5'' | 1.76                     | 0.47              |
| 35:BA:2389:G:C5'   | 35:BA:2390:U:H5'  | 2.43                     | 0.47              |
| 35:BA:286:C:H2'    | 35:BA:287:C:C6    | 2.49                     | 0.47              |
| 36:BB:44:G:H1'     | 36:BB:47:C:N4     | 2.28                     | 0.47              |
| 37:BC:17:PRO:HG2   | 37:BC:18:ASN:H    | 1.79                     | 0.47              |
| 37:BC:180:SER:O    | 37:BC:181:PHE:O   | 2.33                     | 0.47              |
| 37:BC:206:LYS:HB3  | 37:BC:206:LYS:HZ3 | 1.79                     | 0.47              |
| 38:BD:26:LYS:O     | 38:BD:27:THR:HB   | 2.14                     | 0.47              |
| 38:BD:76:PRO:HG2   | 38:BD:98:VAL:CG2  | 2.43                     | 0.47              |
| 39:BE:52:LEU:HD21  | 52:BT:1:MET:HE1   | 1.96                     | 0.47              |
| 41:BG:135:LEU:C    | 41:BG:137:GLU:N   | 2.68                     | 0.47              |
| 41:BG:152:LEU:HD23 | 41:BG:152:LEU:N   | 2.25                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:BG:66:GLN:HE21 | 41:BG:92:VAL:CG2   | 2.26                     | 0.47              |
| 41:BG:5:VAL:HG21  | 41:BG:8:LYS:NZ     | 2.29                     | 0.47              |
| 42:BH:13:LYS:O    | 42:BH:15:VAL:HG22  | 2.15                     | 0.47              |
| 43:BJ:69:UNK:O    | 43:BJ:70:UNK:C     | 2.62                     | 0.47              |
| 45:BL:59:UNK:C    | 45:BL:61:UNK:N     | 2.75                     | 0.47              |
| 49:BQ:33:GLY:HA2  | 49:BQ:105:GLU:HA   | 1.96                     | 0.47              |
| 52:BT:123:GLN:O   | 52:BT:127:ALA:HB3  | 2.13                     | 0.47              |
| 53:BU:32:PHE:O    | 53:BU:36:ARG:HB2   | 2.14                     | 0.47              |
| 55:BW:24:ILE:HG21 | 55:BW:36:LEU:CD1   | 2.44                     | 0.47              |
| 56:BX:8:ILE:HD11  | 56:BX:42:ALA:CB    | 2.34                     | 0.47              |
| 1:AA:1073:U:O2'   | 1:AA:1074:G:C5'    | 2.58                     | 0.47              |
| 1:AA:1368:G:C2'   | 1:AA:1369:C:C5'    | 2.83                     | 0.47              |
| 1:AA:197:A:C5     | 1:AA:221:C:C4'     | 2.95                     | 0.47              |
| 1:AA:342:C:C2'    | 1:AA:343:U:H5'     | 2.43                     | 0.47              |
| 1:AA:563:A:C2     | 1:AA:567:G:C5      | 3.03                     | 0.47              |
| 1:AA:867:G:C6     | 1:AA:868:C:C4      | 3.02                     | 0.47              |
| 4:AD:150:GLU:C    | 4:AD:152:SER:N     | 2.67                     | 0.47              |
| 4:AD:70:ILE:HG23  | 4:AD:74:GLN:HB2    | 1.96                     | 0.47              |
| 8:AH:30:ARG:CZ    | 8:AH:30:ARG:HB3    | 2.44                     | 0.47              |
| 9:AI:17:VAL:O     | 9:AI:17:VAL:HG13   | 2.15                     | 0.47              |
| 10:AJ:3:LYS:HB3   | 10:AJ:4:ILE:CD1    | 2.45                     | 0.47              |
| 13:AM:83:ASP:CG   | 13:AM:84:ILE:H     | 2.17                     | 0.47              |
| 15:AO:39:LEU:HD13 | 15:AO:56:LEU:CB    | 2.43                     | 0.47              |
| 24:AY:550:MET:CE  | 24:AY:563:ILE:HD11 | 2.44                     | 0.47              |
| 25:B0:4:LYS:O     | 25:B0:5:LYS:O      | 2.31                     | 0.47              |
| 25:B0:61:ALA:HB2  | 25:B0:81:VAL:HG21  | 1.96                     | 0.47              |
| 26:B1:20:ARG:HH11 | 26:B1:20:ARG:HG2   | 1.79                     | 0.47              |
| 29:B4:59:PHE:O    | 29:B4:59:PHE:CD1   | 2.66                     | 0.47              |
| 29:B4:66:SER:O    | 29:B4:69:LYS:HG2   | 2.14                     | 0.47              |
| 35:BA:1036:G:N1   | 35:BA:1120:G:C6    | 2.82                     | 0.47              |
| 35:BA:1151:G:H2'  | 35:BA:1152:C:H6    | 1.79                     | 0.47              |
| 35:BA:2052:G:O4'  | 39:BE:142:GLY:HA3  | 2.14                     | 0.47              |
| 35:BA:2110:G:H8   | 35:BA:2110:G:OP2   | 1.96                     | 0.47              |
| 35:BA:2401:U:HO2' | 35:BA:2402:C:P     | 2.37                     | 0.47              |
| 35:BA:527:C:O2    | 35:BA:527:C:O4'    | 2.30                     | 0.47              |
| 35:BA:602:G:O6    | 35:BA:654(T):C:C2  | 2.67                     | 0.47              |
| 35:BA:717:G:H2'   | 35:BA:718:A:O4'    | 2.15                     | 0.47              |
| 35:BA:882:G:N2    | 35:BA:895:U:C2     | 2.82                     | 0.47              |
| 35:BA:7:G:O2'     | 35:BA:8:A:H5'      | 2.15                     | 0.47              |
| 37:BC:20:VAL:O    | 37:BC:21:TYR:CB    | 2.58                     | 0.47              |
| 40:BF:20:LEU:HD13 | 40:BF:203:GLN:OE1  | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BK:4:UNK:O      | 44:BK:5:UNK:C      | 2.62                     | 0.47              |
| 46:BN:119:ARG:HH11 | 46:BN:119:ARG:HG3  | 1.77                     | 0.47              |
| 35:BA:1652:A:H62   | 50:BR:11:ASN:ND2   | 2.12                     | 0.47              |
| 51:BS:24:LEU:O     | 51:BS:85:VAL:HB    | 2.15                     | 0.47              |
| 53:BU:74:LEU:C     | 53:BU:74:LEU:HD12  | 2.35                     | 0.47              |
| 55:BW:24:ILE:HG21  | 55:BW:36:LEU:HD13  | 1.96                     | 0.47              |
| 55:BW:5:ALA:HB2    | 55:BW:54:ALA:HB2   | 1.96                     | 0.47              |
| 58:BZ:151:HIS:CB   | 58:BZ:171:ILE:H    | 2.27                     | 0.47              |
| 1:AA:1381:U:H5     | 1:AA:1382:C:C4     | 2.31                     | 0.47              |
| 1:AA:1392:G:N2     | 1:AA:1502:A:H8     | 2.12                     | 0.47              |
| 1:AA:1400:C:C4'    | 1:AA:1401:G:OP2    | 2.56                     | 0.47              |
| 1:AA:177:C:H2'     | 1:AA:178:C:H6      | 1.78                     | 0.47              |
| 1:AA:605:U:O2'     | 1:AA:606:G:H5'     | 2.14                     | 0.47              |
| 1:AA:863:U:O2      | 1:AA:863:U:C4'     | 2.62                     | 0.47              |
| 2:AB:46:LYS:HA     | 2:AB:49:GLU:OE1    | 2.15                     | 0.47              |
| 7:AG:22:LEU:CD2    | 7:AG:101:LEU:HD11  | 2.45                     | 0.47              |
| 1:AA:1298:C:H2'    | 7:AG:114:ARG:HH12  | 1.78                     | 0.47              |
| 10:AJ:34:VAL:CG2   | 10:AJ:74:ILE:HG22  | 2.32                     | 0.47              |
| 24:AY:164:MET:O    | 24:AY:180:VAL:HG22 | 2.14                     | 0.47              |
| 24:AY:614:GLU:CA   | 24:AY:617:MET:HE3  | 2.39                     | 0.47              |
| 27:B2:4:SER:OG     | 27:B2:5:GLU:N      | 2.48                     | 0.47              |
| 29:B4:16:CYS:CB    | 29:B4:19:GLY:O     | 2.62                     | 0.47              |
| 33:B8:41:ILE:HG12  | 33:B8:41:ILE:O     | 2.14                     | 0.47              |
| 35:BA:1133:U:O2    | 35:BA:1137:G:H5''  | 2.15                     | 0.47              |
| 35:BA:201:C:C2'    | 35:BA:202:U:H5'    | 2.45                     | 0.47              |
| 35:BA:325:G:H2'    | 35:BA:326:G:C8     | 2.46                     | 0.47              |
| 35:BA:27:G:C2      | 35:BA:512:G:H2'    | 2.48                     | 0.47              |
| 35:BA:738:G:C6     | 35:BA:739:G:C2     | 3.02                     | 0.47              |
| 35:BA:806:C:P      | 48:BP:39:LYS:HG3   | 2.53                     | 0.47              |
| 37:BC:75:VAL:HG12  | 37:BC:113:ALA:HB3  | 1.97                     | 0.47              |
| 37:BC:129:GLY:C    | 37:BC:131:ILE:N    | 2.67                     | 0.47              |
| 37:BC:42:VAL:CG1   | 37:BC:43:GLU:H     | 2.27                     | 0.47              |
| 37:BC:80:LYS:O     | 37:BC:83:LYS:HB3   | 2.14                     | 0.47              |
| 39:BE:117:MET:HE3  | 39:BE:136:ARG:HA   | 1.94                     | 0.47              |
| 40:BF:181:LEU:HD23 | 40:BF:202:PHE:HD1  | 1.79                     | 0.47              |
| 40:BF:53:THR:HG22  | 40:BF:56:GLU:OE1   | 2.14                     | 0.47              |
| 41:BG:137:GLU:CD   | 41:BG:154:GLY:H    | 2.18                     | 0.47              |
| 42:BH:153:LYS:CG   | 42:BH:154:PRO:HD2  | 2.44                     | 0.47              |
| 49:BQ:3:MET:HB2    | 49:BQ:4:PRO:HD2    | 1.95                     | 0.47              |
| 35:BA:993:G:OP1    | 53:BU:50:ARG:NH1   | 2.48                     | 0.47              |
| 56:BX:32:PRO:HA    | 56:BX:77:LYS:HB2   | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:183:LEU:HD11 | 58:BZ:186:GLU:HA   | 1.96                     | 0.47              |
| 1:AA:1133:G:C4     | 1:AA:1142:G:N2     | 2.81                     | 0.47              |
| 1:AA:431:A:O2'     | 1:AA:432:A:H5'     | 2.14                     | 0.47              |
| 1:AA:490:G:H2'     | 1:AA:491:G:C8      | 2.38                     | 0.47              |
| 1:AA:563:A:N3      | 1:AA:563:A:C2'     | 2.77                     | 0.47              |
| 1:AA:646:U:H2'     | 1:AA:647:C:C6      | 2.49                     | 0.47              |
| 1:AA:839:U:O2      | 1:AA:839:U:C2'     | 2.61                     | 0.47              |
| 1:AA:868:C:C2'     | 1:AA:869:G:O5'     | 2.62                     | 0.47              |
| 7:AG:116:ALA:HA    | 7:AG:119:ARG:NH1   | 2.30                     | 0.47              |
| 7:AG:33:ASP:C      | 7:AG:35:LYS:H      | 2.17                     | 0.47              |
| 7:AG:49:ILE:O      | 7:AG:50:ILE:CB     | 2.61                     | 0.47              |
| 7:AG:69:VAL:O      | 7:AG:69:VAL:HG22   | 2.14                     | 0.47              |
| 24:AY:512:ILE:N    | 24:AY:512:ILE:HD13 | 2.29                     | 0.47              |
| 24:AY:584:ILE:HG22 | 24:AY:588:MET:CE   | 2.43                     | 0.47              |
| 25:B0:52:GLY:C     | 25:B0:60:PHE:CE1   | 2.88                     | 0.47              |
| 33:B8:4:MET:HB2    | 35:BA:592:G:O2'    | 2.14                     | 0.47              |
| 33:B8:60:LEU:C     | 33:B8:61:LEU:HD12  | 2.35                     | 0.47              |
| 34:B9:17:ILE:CG2   | 34:B9:18:ARG:H     | 2.25                     | 0.47              |
| 34:B9:29:ASN:ND2   | 34:B9:32:HIS:CE1   | 2.83                     | 0.47              |
| 35:BA:1023:U:C2'   | 35:BA:1024:G:C5'   | 2.72                     | 0.47              |
| 35:BA:108:U:H2'    | 35:BA:109:G:C8     | 2.46                     | 0.47              |
| 35:BA:1097:U:C2'   | 35:BA:1098:A:H5'   | 2.43                     | 0.47              |
| 35:BA:1132:A:O2'   | 35:BA:1133:U:H5'   | 2.15                     | 0.47              |
| 35:BA:1800:C:H5'   | 38:BD:147:LEU:HD21 | 1.96                     | 0.47              |
| 35:BA:1885:A:H8    | 35:BA:1885:A:H5'   | 1.79                     | 0.47              |
| 35:BA:1992:G:C2'   | 35:BA:1993:U:OP2   | 2.62                     | 0.47              |
| 35:BA:2134:A:C8    | 35:BA:2158:A:C2    | 3.00                     | 0.47              |
| 22:AV:76:A:H8      | 35:BA:2394:C:H42   | 1.60                     | 0.47              |
| 35:BA:2557:G:C2'   | 35:BA:2558:C:H5'   | 2.44                     | 0.47              |
| 35:BA:2610:C:O2'   | 35:BA:2611:U:OP1   | 2.32                     | 0.47              |
| 35:BA:271(Q):G:O2' | 35:BA:271(R):G:P   | 2.72                     | 0.47              |
| 35:BA:363:G:H2'    | 35:BA:363(A):A:H8  | 1.79                     | 0.47              |
| 35:BA:39:C:C2'     | 35:BA:40:C:C5'     | 2.91                     | 0.47              |
| 35:BA:620:G:H4'    | 35:BA:621:A:H5''   | 1.97                     | 0.47              |
| 35:BA:709:U:H2'    | 35:BA:710:G:C8     | 2.49                     | 0.47              |
| 38:BD:131:LEU:N    | 38:BD:131:LEU:HD12 | 2.28                     | 0.47              |
| 39:BE:61:ARG:C     | 39:BE:63:LEU:H     | 2.16                     | 0.47              |
| 39:BE:2:LYS:HD3    | 39:BE:95:ILE:CG2   | 2.45                     | 0.47              |
| 40:BF:81:PRO:HB3   | 40:BF:89:VAL:HG23  | 1.96                     | 0.47              |
| 41:BG:7:LEU:HB2    | 41:BG:104:GLU:CG   | 2.43                     | 0.47              |
| 41:BG:77:ILE:CG2   | 41:BG:80:PHE:H     | 2.28                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:BT:90:GLN:CB   | 52:BT:121:ILE:HG12 | 2.44                     | 0.47              |
| 53:BU:54:LYS:O    | 53:BU:58:ARG:HG3   | 2.15                     | 0.47              |
| 1:AA:1151:A:C4    | 1:AA:1152:A:C5     | 3.02                     | 0.47              |
| 1:AA:1487:G:C2'   | 1:AA:1488:G:H5'    | 2.45                     | 0.47              |
| 1:AA:188:C:O5'    | 1:AA:188:C:H6      | 1.97                     | 0.47              |
| 1:AA:425:G:O2'    | 1:AA:426:G:H5'     | 2.15                     | 0.47              |
| 3:AC:190:ARG:NH1  | 3:AC:190:ARG:HG3   | 2.30                     | 0.47              |
| 7:AG:89:MET:HE1   | 7:AG:155:ARG:HB3   | 1.96                     | 0.47              |
| 1:AA:963:G:N2     | 10:AJ:55:LYS:HD3   | 2.29                     | 0.47              |
| 13:AM:32:GLU:O    | 13:AM:35:GLU:HG2   | 2.14                     | 0.47              |
| 19:AS:51:VAL:HG21 | 19:AS:71:LEU:HB3   | 1.95                     | 0.47              |
| 24:AY:186:TYR:N   | 24:AY:186:TYR:CD1  | 2.82                     | 0.47              |
| 24:AY:488:THR:O   | 24:AY:516:PRO:HG3  | 2.14                     | 0.47              |
| 24:AY:550:MET:SD  | 24:AY:563:ILE:HD11 | 2.54                     | 0.47              |
| 25:B0:12:ASN:HA   | 25:B0:14:ARG:NH1   | 2.30                     | 0.47              |
| 27:B2:53:LEU:O    | 27:B2:53:LEU:HD23  | 2.14                     | 0.47              |
| 28:B3:22:ALA:CA   | 28:B3:46:ASN:HD22  | 2.26                     | 0.47              |
| 29:B4:21:VAL:O    | 29:B4:22:ILE:C     | 2.52                     | 0.47              |
| 29:B4:38:LYS:HG2  | 29:B4:47:GLN:OE1   | 2.15                     | 0.47              |
| 31:B6:17:LYS:C    | 31:B6:18:ARG:HD2   | 2.35                     | 0.47              |
| 35:BA:1198:U:H2'  | 35:BA:1199:U:C6    | 2.50                     | 0.47              |
| 35:BA:1223:G:C2   | 35:BA:1227:G:C5    | 3.03                     | 0.47              |
| 35:BA:1678:G:O5'  | 35:BA:1678:G:H8    | 1.98                     | 0.47              |
| 35:BA:1805:U:O2'  | 35:BA:1806:C:C5'   | 2.47                     | 0.47              |
| 35:BA:2147:G:H2'  | 35:BA:2148:G:C4'   | 2.44                     | 0.47              |
| 35:BA:2175:C:H2'  | 35:BA:2176:A:H8    | 1.78                     | 0.47              |
| 35:BA:2193:G:C4   | 35:BA:2194:G:C8    | 3.02                     | 0.47              |
| 35:BA:2364:C:C2'  | 35:BA:2365:G:H5'   | 2.45                     | 0.47              |
| 35:BA:2615:U:H2'  | 35:BA:2616:C:H6    | 1.79                     | 0.47              |
| 32:B7:40:TRP:CD2  | 35:BA:459:U:H5''   | 2.49                     | 0.47              |
| 35:BA:527:C:H1'   | 35:BA:528:A:C8     | 2.49                     | 0.47              |
| 35:BA:90:U:HO2'   | 35:BA:92:A:P       | 2.37                     | 0.47              |
| 36:BB:13:A:N1     | 36:BB:69:G:O2'     | 2.40                     | 0.47              |
| 39:BE:61:ARG:O    | 39:BE:63:LEU:N     | 2.41                     | 0.47              |
| 40:BF:198:ALA:O   | 40:BF:201:VAL:HG12 | 2.15                     | 0.47              |
| 40:BF:20:LEU:HB3  | 40:BF:23:ASP:CG    | 2.35                     | 0.47              |
| 41:BG:83:ARG:C    | 41:BG:85:GLY:N     | 2.68                     | 0.47              |
| 43:BJ:51:UNK:O    | 43:BJ:87:UNK:HA    | 2.14                     | 0.47              |
| 46:BN:15:LEU:O    | 46:BN:136:GLU:HA   | 2.15                     | 0.47              |
| 47:BO:11:ALA:O    | 47:BO:98:VAL:HG23  | 2.14                     | 0.47              |
| 48:BP:52:GLU:CG   | 48:BP:57:THR:HG22  | 2.35                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BT:13:ARG:NE    | 52:BT:13:ARG:HA    | 2.27                     | 0.47              |
| 53:BU:61:TRP:O     | 53:BU:65:ILE:HD13  | 2.15                     | 0.47              |
| 35:BA:747:U:H1'    | 55:BW:92:ARG:NH2   | 2.29                     | 0.47              |
| 58:BZ:102:LEU:HD12 | 58:BZ:121:HIS:O    | 2.14                     | 0.47              |
| 58:BZ:20:ARG:HH11  | 58:BZ:20:ARG:HB3   | 1.80                     | 0.47              |
| 49:BQ:141:GLN:CG   | 58:BZ:72:ARG:CZ    | 2.93                     | 0.47              |
| 1:AA:1476:G:H2'    | 1:AA:1477:C:C6     | 2.50                     | 0.47              |
| 1:AA:187:C:C2'     | 1:AA:188:C:H5'     | 2.44                     | 0.47              |
| 1:AA:339:C:H2'     | 1:AA:340:U:H6      | 1.80                     | 0.47              |
| 1:AA:360:A:H2'     | 1:AA:361:G:C5'     | 2.45                     | 0.47              |
| 1:AA:360:A:H2'     | 1:AA:361:G:C8      | 2.50                     | 0.47              |
| 1:AA:491:G:C2'     | 1:AA:492:G:O5'     | 2.62                     | 0.47              |
| 1:AA:544:G:C2'     | 1:AA:545:C:O5'     | 2.63                     | 0.47              |
| 1:AA:954:G:H2'     | 1:AA:955:U:H6      | 1.78                     | 0.47              |
| 2:AB:21:ARG:O      | 2:AB:23:ARG:N      | 2.40                     | 0.47              |
| 5:AE:82:VAL:HG21   | 5:AE:138:ALA:HA    | 1.97                     | 0.47              |
| 7:AG:15:ASP:HB3    | 7:AG:19:GLY:C      | 2.34                     | 0.47              |
| 1:AA:933:G:OP2     | 7:AG:3:ARG:HB2     | 2.14                     | 0.47              |
| 11:AK:57:THR:OG1   | 11:AK:58:PRO:HD2   | 2.14                     | 0.47              |
| 12:AL:47:LYS:O     | 12:AL:48:PRO:C     | 2.53                     | 0.47              |
| 24:AY:126:GLU:O    | 24:AY:129:LYS:N    | 2.37                     | 0.47              |
| 24:AY:35:TYR:OH    | 24:AY:266:ASN:HB3  | 2.14                     | 0.47              |
| 24:AY:583:LYS:HD3  | 24:AY:583:LYS:C    | 2.35                     | 0.47              |
| 19:AS:20:LEU:CD1   | 29:B4:61:ARG:HH21  | 2.28                     | 0.47              |
| 35:BA:1197:G:O2'   | 35:BA:1198:U:H5'   | 2.14                     | 0.47              |
| 35:BA:1288:U:C2    | 35:BA:1327:C:O2    | 2.67                     | 0.47              |
| 35:BA:15:G:C4      | 35:BA:16:G:C8      | 3.03                     | 0.47              |
| 35:BA:1893:C:C2'   | 35:BA:1894:C:H5'   | 2.44                     | 0.47              |
| 35:BA:2009:G:C2'   | 35:BA:2010:G:H5''  | 2.43                     | 0.47              |
| 35:BA:2352:A:H2'   | 35:BA:2353:G:O4'   | 2.14                     | 0.47              |
| 35:BA:2505:G:O6    | 35:BA:2576:G:H2'   | 2.15                     | 0.47              |
| 35:BA:576:U:H2'    | 35:BA:577:G:C8     | 2.50                     | 0.47              |
| 35:BA:612:C:C2'    | 35:BA:613:G:C5'    | 2.71                     | 0.47              |
| 35:BA:628:G:H2'    | 35:BA:629:G:C5'    | 2.42                     | 0.47              |
| 35:BA:603:A:C8     | 35:BA:655:A:C6     | 3.03                     | 0.47              |
| 35:BA:753:C:H2'    | 35:BA:754:C:H6     | 1.78                     | 0.47              |
| 36:BB:37:C:H2'     | 36:BB:38:C:H5'     | 1.97                     | 0.47              |
| 37:BC:105:LEU:H    | 37:BC:105:LEU:HD22 | 1.80                     | 0.47              |
| 38:BD:186:HIS:CD2  | 38:BD:188:GLU:HB2  | 2.50                     | 0.47              |
| 40:BF:3:GLU:HA     | 40:BF:24:LEU:CG    | 2.44                     | 0.47              |
| 41:BG:28:VAL:HG12  | 41:BG:28:VAL:O     | 2.13                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BG:5:VAL:HG11   | 41:BG:8:LYS:HB2   | 1.96                     | 0.47              |
| 49:BQ:1:MET:HE2    | 49:BQ:1:MET:HA    | 1.97                     | 0.47              |
| 51:BS:93:LYS:O     | 51:BS:93:LYS:HG3  | 2.14                     | 0.47              |
| 52:BT:48:ILE:HD12  | 52:BT:48:ILE:H    | 1.79                     | 0.47              |
| 47:BO:77:ILE:CD1   | 52:BT:74:ARG:HD3  | 2.44                     | 0.47              |
| 52:BT:25:GLY:CA    | 52:BT:92:GLY:HA2  | 2.45                     | 0.47              |
| 54:BV:68:LYS:HD2   | 54:BV:69:LYS:H    | 1.80                     | 0.47              |
| 56:BX:23:GLU:CD    | 56:BX:23:GLU:H    | 2.18                     | 0.47              |
| 58:BZ:185:GLU:O    | 58:BZ:186:GLU:C   | 2.50                     | 0.47              |
| 1:AA:1073:U:H2'    | 1:AA:1074:G:C5'   | 2.32                     | 0.47              |
| 1:AA:1142:G:C8     | 1:AA:1143:G:C8    | 3.03                     | 0.47              |
| 1:AA:123:C:H2'     | 1:AA:124:G:C8     | 2.50                     | 0.47              |
| 1:AA:160:A:H1'     | 1:AA:344:A:C2     | 2.49                     | 0.47              |
| 1:AA:353:A:H2'     | 1:AA:354:G:OP2    | 2.15                     | 0.47              |
| 1:AA:564:C:C4      | 1:AA:565:U:C4     | 3.02                     | 0.47              |
| 1:AA:590:C:OP1     | 8:AH:30:ARG:N     | 2.43                     | 0.47              |
| 1:AA:713:G:H2'     | 1:AA:714:G:C8     | 2.49                     | 0.47              |
| 1:AA:961:U:C2'     | 1:AA:961:U:OP1    | 2.63                     | 0.47              |
| 3:AC:207:VAL:HG12  | 3:AC:207:VAL:O    | 2.14                     | 0.47              |
| 3:AC:91:LEU:CB     | 3:AC:99:VAL:HG21  | 2.44                     | 0.47              |
| 6:AF:71:ARG:NH1    | 6:AF:71:ARG:HG3   | 2.29                     | 0.47              |
| 7:AG:69:VAL:HG11   | 7:AG:104:LEU:HD13 | 1.96                     | 0.47              |
| 9:AI:50:LEU:HD23   | 9:AI:85:LEU:HD23  | 1.97                     | 0.47              |
| 9:AI:6:GLY:O       | 9:AI:17:VAL:HG12  | 2.14                     | 0.47              |
| 18:AR:56:THR:HB    | 18:AR:58:LEU:HD12 | 1.94                     | 0.47              |
| 20:AT:22:ARG:O     | 20:AT:26:ASN:ND2  | 2.47                     | 0.47              |
| 7:AG:81:GLY:C      | 23:AX:12:A:O3'    | 2.53                     | 0.47              |
| 24:AY:238:THR:HG23 | 24:AY:241:GLU:H   | 1.79                     | 0.47              |
| 24:AY:588:MET:HA   | 24:AY:591:LYS:HB3 | 1.96                     | 0.47              |
| 24:AY:584:ILE:O    | 24:AY:588:MET:HE2 | 2.14                     | 0.47              |
| 26:B1:24:ALA:HB3   | 26:B1:27:GLU:HG3  | 1.97                     | 0.47              |
| 28:B3:10:LYS:HB3   | 28:B3:53:LEU:HD23 | 1.95                     | 0.47              |
| 30:B5:54:GLY:O     | 30:B5:55:ARG:C    | 2.53                     | 0.47              |
| 33:B8:29:LYS:HD3   | 33:B8:44:LYS:HB3  | 1.95                     | 0.47              |
| 35:BA:1779:U:H6    | 35:BA:1779:U:H3'  | 1.79                     | 0.47              |
| 35:BA:528:A:C2     | 35:BA:2043:C:H5'  | 2.47                     | 0.47              |
| 35:BA:2148:G:O2'   | 35:BA:2149:G:H5'  | 2.14                     | 0.47              |
| 35:BA:2783:G:H2'   | 35:BA:2784:C:H6   | 1.79                     | 0.47              |
| 35:BA:582:G:H2'    | 35:BA:583:G:H8    | 1.78                     | 0.47              |
| 35:BA:796:C:H2'    | 35:BA:797:C:H6    | 1.77                     | 0.47              |
| 35:BA:902:C:H2'    | 35:BA:903:C:H6    | 1.76                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BF:82:ILE:H    | 40:BF:82:ILE:HG12  | 1.32                     | 0.47              |
| 48:BP:46:LYS:HG2  | 48:BP:51:PHE:CG    | 2.49                     | 0.47              |
| 51:BS:56:LEU:HD23 | 51:BS:57:LYS:O     | 2.14                     | 0.47              |
| 52:BT:133:GLU:OE1 | 52:BT:136:GLN:HB3  | 2.15                     | 0.47              |
| 57:BY:81:LYS:HD3  | 57:BY:97:ARG:CG    | 2.39                     | 0.47              |
| 1:AA:1157:A:H4'   | 1:AA:1158:C:C5'    | 2.43                     | 0.47              |
| 1:AA:1384:C:C2    | 1:AA:1385:G:C8     | 3.03                     | 0.47              |
| 1:AA:412:A:H5'    | 1:AA:413:G:OP1     | 2.15                     | 0.47              |
| 1:AA:444:C:H2'    | 1:AA:445:G:C8      | 2.50                     | 0.47              |
| 1:AA:751:U:C2'    | 1:AA:752:G:H5'     | 2.45                     | 0.47              |
| 1:AA:774:G:H2'    | 1:AA:775:G:O5'     | 2.15                     | 0.47              |
| 1:AA:820:U:H4'    | 1:AA:821:G:OP2     | 2.15                     | 0.47              |
| 1:AA:961:U:O2'    | 1:AA:962:C:P       | 2.73                     | 0.47              |
| 2:AB:19:HIS:O     | 2:AB:20:GLU:HB2    | 2.14                     | 0.47              |
| 2:AB:20:GLU:CB    | 2:AB:190:THR:OG1   | 2.62                     | 0.47              |
| 3:AC:113:ALA:HA   | 3:AC:116:VAL:HG12  | 1.96                     | 0.47              |
| 9:AI:9:ARG:HG2    | 9:AI:14:VAL:HG13   | 1.96                     | 0.47              |
| 12:AL:24:VAL:O    | 12:AL:24:VAL:HG12  | 2.15                     | 0.47              |
| 12:AL:94:PRO:O    | 12:AL:96:VAL:N     | 2.48                     | 0.47              |
| 19:AS:25:LYS:HG3  | 19:AS:26:GLY:N     | 2.30                     | 0.47              |
| 19:AS:35:SER:C    | 19:AS:37:ARG:N     | 2.67                     | 0.47              |
| 24:AY:319:ASP:OD2 | 24:AY:322:VAL:HG22 | 2.15                     | 0.47              |
| 30:B5:40:LYS:HD3  | 30:B5:46:CYS:CB    | 2.44                     | 0.47              |
| 35:BA:1106:G:H2'  | 35:BA:1107:G:H8    | 1.80                     | 0.47              |
| 35:BA:1133:U:O3'  | 35:BA:1135:C:OP2   | 2.33                     | 0.47              |
| 35:BA:1501:C:H1'  | 38:BD:100:GLY:HA2  | 1.95                     | 0.47              |
| 35:BA:150:C:H2'   | 35:BA:151:C:C6     | 2.50                     | 0.47              |
| 35:BA:1540:U:O2'  | 35:BA:1541:G:OP1   | 2.33                     | 0.47              |
| 35:BA:1995:U:H2'  | 35:BA:1996:C:C6    | 2.50                     | 0.47              |
| 35:BA:2126:A:O2'  | 35:BA:2127:G:O4'   | 2.30                     | 0.47              |
| 35:BA:2337:G:H2'  | 35:BA:2338:G:H8    | 1.80                     | 0.47              |
| 35:BA:2360:A:HO2' | 35:BA:2361:A:P     | 2.37                     | 0.47              |
| 35:BA:2291:U:OP1  | 35:BA:2381:C:H5'   | 2.15                     | 0.47              |
| 35:BA:2401:U:H5'' | 35:BA:2402:C:H5    | 1.79                     | 0.47              |
| 35:BA:285:C:O2'   | 35:BA:286:C:H5'    | 2.15                     | 0.47              |
| 36:BB:3:C:N4      | 36:BB:118:G:H1     | 2.05                     | 0.47              |
| 37:BC:118:PRO:HB3 | 37:BC:121:MET:HG2  | 1.97                     | 0.47              |
| 37:BC:228:HIS:O   | 37:BC:229:SER:HB3  | 2.15                     | 0.47              |
| 38:BD:243:GLY:O   | 38:BD:244:ARG:O    | 2.32                     | 0.47              |
| 38:BD:266:SER:O   | 38:BD:267:SER:O    | 2.33                     | 0.47              |
| 35:BA:2580:U:H5'  | 39:BE:131:ALA:H    | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BE:61:ARG:HG3   | 39:BE:61:ARG:HH11  | 1.79                     | 0.47              |
| 40:BF:192:LEU:HD22 | 40:BF:194:MET:HE2  | 1.96                     | 0.47              |
| 29:B4:35:VAL:HG13  | 41:BG:108:ASN:O    | 2.15                     | 0.47              |
| 41:BG:180:PHE:C    | 41:BG:180:PHE:CD1  | 2.88                     | 0.47              |
| 41:BG:51:ARG:C     | 41:BG:52:ILE:HG13  | 2.33                     | 0.47              |
| 44:BK:88:UNK:HA    | 44:BK:96:UNK:H2    | 1.79                     | 0.47              |
| 46:BN:45:ASN:ND2   | 46:BN:45:ASN:H     | 2.13                     | 0.47              |
| 49:BQ:116:GLU:O    | 49:BQ:120:ILE:HG12 | 2.14                     | 0.47              |
| 1:AA:17:U:H4'      | 1:AA:1080:A:O4'    | 2.15                     | 0.47              |
| 1:AA:1129:C:O3'    | 1:AA:1131:G:OP2    | 2.33                     | 0.47              |
| 1:AA:1283:G:O2'    | 1:AA:1284:C:P      | 2.73                     | 0.47              |
| 1:AA:1346:A:O3'    | 1:AA:1347:G:H4'    | 2.15                     | 0.47              |
| 1:AA:701:C:P       | 1:AA:703:G:H5'     | 2.55                     | 0.47              |
| 2:AB:127:ILE:HD13  | 2:AB:135:GLN:NE2   | 2.29                     | 0.47              |
| 3:AC:121:ALA:O     | 3:AC:124:ILE:HG22  | 2.14                     | 0.47              |
| 3:AC:42:LEU:HD12   | 3:AC:42:LEU:O      | 2.14                     | 0.47              |
| 3:AC:72:LYS:HE3    | 3:AC:74:GLY:H      | 1.80                     | 0.47              |
| 9:AI:114:TYR:HE1   | 10:AJ:59:SER:HA    | 1.80                     | 0.47              |
| 1:AA:539:A:OP2     | 12:AL:115:LYS:HE3  | 2.15                     | 0.47              |
| 13:AM:2:ALA:N      | 13:AM:9:ILE:HG22   | 2.29                     | 0.47              |
| 11:AK:108:ILE:HG21 | 18:AR:88:LYS:HB3   | 1.97                     | 0.47              |
| 24:AY:108:PHE:CE2  | 24:AY:114:VAL:HG22 | 2.50                     | 0.47              |
| 24:AY:428:LEU:HB3  | 24:AY:440:VAL:HG21 | 1.96                     | 0.47              |
| 24:AY:547:GLU:O    | 24:AY:550:MET:HB3  | 2.15                     | 0.47              |
| 24:AY:600:VAL:HG21 | 24:AY:678:GLU:CG   | 2.45                     | 0.47              |
| 25:B0:72:ARG:HB3   | 25:B0:75:LEU:HB2   | 1.96                     | 0.47              |
| 26:B1:84:GLY:O     | 26:B1:90:ILE:HD11  | 2.15                     | 0.47              |
| 29:B4:16:CYS:HB3   | 29:B4:19:GLY:O     | 2.15                     | 0.47              |
| 29:B4:2:LYS:HD2    | 29:B4:6:HIS:CD2    | 2.50                     | 0.47              |
| 31:B6:45:LYS:CB    | 31:B6:45:LYS:NZ    | 2.78                     | 0.47              |
| 33:B8:61:LEU:N     | 33:B8:61:LEU:CD1   | 2.76                     | 0.47              |
| 35:BA:1067:A:C3'   | 35:BA:1068:G:H5''  | 2.45                     | 0.47              |
| 35:BA:1286:A:C4    | 35:BA:1329:U:C4    | 3.03                     | 0.47              |
| 35:BA:1541:G:O2'   | 35:BA:1542:A:C5'   | 2.63                     | 0.47              |
| 35:BA:1542:A:C8    | 35:BA:1544:A:H5'   | 2.50                     | 0.47              |
| 35:BA:2134:A:N6    | 35:BA:2157:G:H1'   | 2.30                     | 0.47              |
| 35:BA:1999:C:H5''  | 35:BA:2723:C:O2'   | 2.15                     | 0.47              |
| 35:BA:2757:A:C2'   | 35:BA:2758:A:O5'   | 2.61                     | 0.47              |
| 35:BA:31:C:C3'     | 35:BA:32:C:C5'     | 2.93                     | 0.47              |
| 32:B7:34:ARG:HD3   | 35:BA:467:G:OP2    | 2.14                     | 0.47              |
| 35:BA:860:U:O4'    | 35:BA:860:U:O2     | 2.31                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BB:53:A:H2'    | 36:BB:53:A:N3     | 2.29                     | 0.47              |
| 37:BC:6:LYS:HA    | 37:BC:9:ARG:NH1   | 2.30                     | 0.47              |
| 37:BC:88:GLU:HA   | 37:BC:92:ALA:CB   | 2.45                     | 0.47              |
| 38:BD:209:ALA:C   | 38:BD:210:GLY:O   | 2.52                     | 0.47              |
| 38:BD:210:GLY:O   | 38:BD:212:SER:N   | 2.46                     | 0.47              |
| 38:BD:21:PHE:HB3  | 38:BD:24:ILE:CG2  | 2.44                     | 0.47              |
| 40:BF:29:ASN:H    | 40:BF:112:MET:CE  | 2.28                     | 0.47              |
| 41:BG:9:ARG:HB3   | 41:BG:13:GLU:OE1  | 2.15                     | 0.47              |
| 41:BG:39:ILE:O    | 41:BG:39:ILE:HG23 | 2.14                     | 0.47              |
| 42:BH:89:ILE:CG1  | 42:BH:89:ILE:O    | 2.62                     | 0.47              |
| 48:BP:18:ARG:O    | 48:BP:20:GLY:N    | 2.48                     | 0.47              |
| 48:BP:34:GLY:O    | 48:BP:35:HIS:CB   | 2.62                     | 0.47              |
| 50:BR:28:LEU:HD23 | 50:BR:28:LEU:O    | 2.15                     | 0.47              |
| 52:BT:106:SER:O   | 52:BT:107:ASP:HB3 | 2.15                     | 0.47              |
| 35:BA:2848:G:H3'  | 52:BT:95:ARG:O    | 2.14                     | 0.47              |
| 57:BY:95:LYS:HE3  | 57:BY:96:ILE:O    | 2.14                     | 0.47              |
| 1:AA:1036:G:H3'   | 1:AA:1037:C:C6    | 2.49                     | 0.47              |
| 1:AA:1305:G:O2'   | 1:AA:1306:A:C8    | 2.54                     | 0.47              |
| 1:AA:255:G:O6     | 1:AA:266:G:O6     | 2.33                     | 0.47              |
| 1:AA:41:G:O2'     | 1:AA:42:G:H5'     | 2.15                     | 0.47              |
| 1:AA:941:G:H2'    | 1:AA:942:G:O5'    | 2.15                     | 0.47              |
| 1:AA:942:G:C2     | 1:AA:943:U:C5     | 3.03                     | 0.47              |
| 2:AB:96:ARG:HG3   | 2:AB:98:LEU:HD23  | 1.97                     | 0.47              |
| 4:AD:25:ARG:C     | 4:AD:27:TYR:H     | 2.18                     | 0.47              |
| 8:AH:121:ASP:HB2  | 8:AH:125:ARG:HH22 | 1.80                     | 0.47              |
| 25:B0:38:VAL:HG12 | 25:B0:39:ARG:N    | 2.29                     | 0.47              |
| 27:B2:8:LYS:O     | 27:B2:9:GLN:C     | 2.53                     | 0.47              |
| 29:B4:62:ARG:C    | 29:B4:64:GLY:H    | 2.19                     | 0.47              |
| 31:B6:22:ALA:C    | 31:B6:23:THR:HG23 | 2.35                     | 0.47              |
| 35:BA:9:U:O2'     | 35:BA:10:G:P      | 2.73                     | 0.47              |
| 35:BA:1461:G:P    | 35:BA:1461:G:H8   | 2.38                     | 0.47              |
| 35:BA:2236:C:H2'  | 35:BA:2237:G:O4'  | 2.15                     | 0.47              |
| 33:B8:27:THR:CG2  | 35:BA:2361:A:OP1  | 2.59                     | 0.47              |
| 35:BA:614:U:O2    | 35:BA:614:U:O4'   | 2.31                     | 0.47              |
| 35:BA:693:C:C2'   | 35:BA:694:U:O5'   | 2.63                     | 0.47              |
| 35:BA:880:G:H2'   | 35:BA:881:G:C5'   | 2.42                     | 0.47              |
| 36:BB:14:U:OP2    | 36:BB:71:C:H5'    | 2.15                     | 0.47              |
| 38:BD:95:LEU:HD11 | 38:BD:103:ARG:HB2 | 1.97                     | 0.47              |
| 35:BA:1818:U:O4   | 38:BD:154:LYS:HD3 | 2.16                     | 0.47              |
| 41:BG:100:TRP:O   | 41:BG:104:GLU:HB2 | 2.15                     | 0.47              |
| 13:AM:7:VAL:HG22  | 41:BG:147:ASP:OD1 | 2.10                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BH:67:LEU:O     | 42:BH:71:LEU:HD12  | 2.15                     | 0.47              |
| 35:BA:958:U:O4     | 49:BQ:17:LEU:HG    | 2.15                     | 0.47              |
| 50:BR:54:LEU:HB3   | 50:BR:62:ALA:HB1   | 1.97                     | 0.47              |
| 51:BS:49:VAL:HG12  | 51:BS:50:SER:N     | 2.28                     | 0.47              |
| 56:BX:14:SER:O     | 56:BX:15:GLU:C     | 2.54                     | 0.47              |
| 56:BX:57:LEU:HD22  | 56:BX:78:LYS:HB3   | 1.97                     | 0.47              |
| 57:BY:49:VAL:O     | 57:BY:50:ARG:HB2   | 2.14                     | 0.47              |
| 1:AA:1307:U:C2     | 1:AA:1308:U:C5     | 3.02                     | 0.46              |
| 1:AA:1312:G:O2'    | 1:AA:1313:U:H5'    | 2.15                     | 0.46              |
| 1:AA:1388:C:HO2'   | 1:AA:1389:C:H5'    | 1.75                     | 0.46              |
| 1:AA:1498:U:H4'    | 1:AA:1499:A:C5'    | 2.44                     | 0.46              |
| 1:AA:198:G:C6      | 1:AA:220:G:C5      | 3.00                     | 0.46              |
| 1:AA:423:G:C2'     | 1:AA:424:G:H5'     | 2.45                     | 0.46              |
| 1:AA:679:C:H2'     | 1:AA:680:C:C6      | 2.50                     | 0.46              |
| 1:AA:688:G:N1      | 1:AA:700:G:C4      | 2.83                     | 0.46              |
| 1:AA:774:G:C2'     | 1:AA:775:G:O5'     | 2.63                     | 0.46              |
| 1:AA:949:A:C3'     | 1:AA:950:U:C5'     | 2.91                     | 0.46              |
| 2:AB:115:LEU:CD1   | 2:AB:149:LEU:HB3   | 2.45                     | 0.46              |
| 2:AB:115:LEU:HD23  | 2:AB:115:LEU:C     | 2.35                     | 0.46              |
| 2:AB:93:VAL:HG22   | 2:AB:93:VAL:O      | 2.14                     | 0.46              |
| 3:AC:17:ASP:CG     | 3:AC:18:TRP:H      | 2.18                     | 0.46              |
| 3:AC:72:LYS:HE3    | 3:AC:74:GLY:CA     | 2.45                     | 0.46              |
| 4:AD:13:ARG:HG2    | 4:AD:33:MET:CE     | 2.45                     | 0.46              |
| 10:AJ:33:GLN:CG    | 10:AJ:75:ILE:HD11  | 2.45                     | 0.46              |
| 24:AY:108:PHE:HE2  | 24:AY:114:VAL:HG22 | 1.80                     | 0.46              |
| 24:AY:148:LEU:O    | 24:AY:152:THR:HB   | 2.14                     | 0.46              |
| 24:AY:343:ASN:O    | 24:AY:347:GLY:N    | 2.48                     | 0.46              |
| 24:AY:36:THR:OG1   | 24:AY:37:GLY:N     | 2.49                     | 0.46              |
| 24:AY:600:VAL:HG21 | 24:AY:678:GLU:CD   | 2.36                     | 0.46              |
| 24:AY:86:GLY:O     | 24:AY:117:GLN:HG3  | 2.15                     | 0.46              |
| 28:B3:5:LYS:HE2    | 28:B3:34:GLU:CD    | 2.35                     | 0.46              |
| 28:B3:9:VAL:CG2    | 28:B3:55:ARG:HD2   | 2.44                     | 0.46              |
| 29:B4:65:ASP:O     | 29:B4:67:TYR:N     | 2.48                     | 0.46              |
| 30:B5:51:TYR:HB3   | 30:B5:54:GLY:HA3   | 1.97                     | 0.46              |
| 32:B7:34:ARG:CG    | 32:B7:34:ARG:HH11  | 2.20                     | 0.46              |
| 35:BA:1113:U:H2'   | 35:BA:1114:G:H8    | 1.79                     | 0.46              |
| 35:BA:1422:G:H2'   | 35:BA:1423:G:C8    | 2.49                     | 0.46              |
| 35:BA:221:A:N7     | 35:BA:266:G:C6     | 2.83                     | 0.46              |
| 35:BA:2713:A:C3'   | 35:BA:2714:G:H5''  | 2.43                     | 0.46              |
| 35:BA:33:U:O4      | 35:BA:446:G:O2'    | 2.17                     | 0.46              |
| 35:BA:860:U:H2'    | 35:BA:861:A:H5'    | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BB:54:G:O2'     | 36:BB:55:U:H5'     | 2.15                     | 0.46              |
| 36:BB:8:U:C6       | 36:BB:8:U:H5'      | 2.35                     | 0.46              |
| 37:BC:176:VAL:HG12 | 37:BC:176:VAL:O    | 2.15                     | 0.46              |
| 35:BA:2580:U:H5'   | 39:BE:131:ALA:N    | 2.30                     | 0.46              |
| 40:BF:178:PRO:HG2  | 40:BF:179:GLU:OE1  | 2.15                     | 0.46              |
| 40:BF:192:LEU:HD22 | 40:BF:194:MET:HG3  | 1.97                     | 0.46              |
| 41:BG:56:ALA:HB2   | 41:BG:153:ARG:CZ   | 2.45                     | 0.46              |
| 41:BG:52:ILE:HD12  | 41:BG:53:LEU:N     | 2.30                     | 0.46              |
| 42:BH:85:LYS:HZ2   | 42:BH:145:ALA:HA   | 1.80                     | 0.46              |
| 44:BK:112:UNK:O    | 44:BK:113:UNK:C    | 2.62                     | 0.46              |
| 46:BN:37:LYS:HG3   | 46:BN:42:TRP:CE3   | 2.50                     | 0.46              |
| 46:BN:58:ASP:O     | 46:BN:60:ILE:N     | 2.48                     | 0.46              |
| 48:BP:146:VAL:CG2  | 48:BP:147:LEU:H    | 2.07                     | 0.46              |
| 52:BT:16:ARG:HH12  | 52:BT:19:LEU:HG    | 1.80                     | 0.46              |
| 52:BT:27:THR:O     | 52:BT:28:VAL:CB    | 2.63                     | 0.46              |
| 52:BT:90:GLN:HB3   | 52:BT:121:ILE:HG12 | 1.96                     | 0.46              |
| 54:BV:19:LYS:NZ    | 54:BV:20:LEU:N     | 2.62                     | 0.46              |
| 58:BZ:20:ARG:CB    | 58:BZ:20:ARG:HH11  | 2.27                     | 0.46              |
| 1:AA:1046:A:H2'    | 1:AA:1047:G:H5'    | 1.97                     | 0.46              |
| 1:AA:1151:A:N1     | 1:AA:1152:A:C6     | 2.83                     | 0.46              |
| 1:AA:1180:A:O5'    | 1:AA:1180:A:H8     | 1.99                     | 0.46              |
| 1:AA:1296:C:C5'    | 1:AA:1302:U:O4     | 2.63                     | 0.46              |
| 1:AA:29:G:O2'      | 1:AA:30:U:H5'      | 2.15                     | 0.46              |
| 1:AA:389:A:N3      | 1:AA:389:A:H2'     | 2.30                     | 0.46              |
| 1:AA:736:C:H2'     | 1:AA:737:A:C8      | 2.50                     | 0.46              |
| 1:AA:789:U:H6      | 1:AA:789:U:O5'     | 1.98                     | 0.46              |
| 1:AA:859:A:C2'     | 1:AA:860:A:C5'     | 2.87                     | 0.46              |
| 1:AA:865:A:C5      | 1:AA:866:C:C4      | 3.03                     | 0.46              |
| 2:AB:111:ARG:HD2   | 2:AB:111:ARG:HA    | 1.64                     | 0.46              |
| 2:AB:95:GLN:HE21   | 2:AB:147:LYS:HE2   | 1.80                     | 0.46              |
| 3:AC:31:HIS:O      | 3:AC:34:LEU:N      | 2.49                     | 0.46              |
| 3:AC:84:ILE:HG23   | 3:AC:85:ARG:N      | 2.30                     | 0.46              |
| 3:AC:99:VAL:O      | 3:AC:99:VAL:HG23   | 2.14                     | 0.46              |
| 4:AD:158:ILE:HG22  | 4:AD:181:MET:HE2   | 1.98                     | 0.46              |
| 4:AD:158:ILE:HG22  | 4:AD:181:MET:CE    | 2.45                     | 0.46              |
| 13:AM:66:LEU:CD1   | 13:AM:66:LEU:N     | 2.77                     | 0.46              |
| 15:AO:17:ARG:O     | 15:AO:18:PHE:HB3   | 2.16                     | 0.46              |
| 18:AR:26:LEU:HG    | 18:AR:42:ARG:NH1   | 2.30                     | 0.46              |
| 22:AV:47:U:H3'     | 22:AV:48:C:H5''    | 1.98                     | 0.46              |
| 24:AY:122:TRP:CG   | 24:AY:157:LEU:HD12 | 2.50                     | 0.46              |
| 24:AY:421:GLN:CA   | 24:AY:421:GLN:HE21 | 2.28                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:B4:6:HIS:ND1    | 29:B4:7:PRO:HD2    | 2.30                     | 0.46              |
| 35:BA:1104:C:O5'   | 35:BA:1104:C:H6    | 1.97                     | 0.46              |
| 35:BA:1290:C:H2'   | 35:BA:1291:C:C6    | 2.49                     | 0.46              |
| 35:BA:1416:G:N2    | 35:BA:1417:C:N3    | 2.63                     | 0.46              |
| 35:BA:1434:A:H2'   | 35:BA:1435:G:C8    | 2.50                     | 0.46              |
| 35:BA:1463:C:H2'   | 35:BA:1464:C:C6    | 2.50                     | 0.46              |
| 35:BA:155:U:C3'    | 35:BA:156:U:H5''   | 2.46                     | 0.46              |
| 35:BA:1625:C:H2'   | 35:BA:1626:G:H5'   | 1.97                     | 0.46              |
| 35:BA:1769:G:O6    | 35:BA:1984:G:O6    | 2.34                     | 0.46              |
| 35:BA:570:G:H2'    | 35:BA:2030:A:N7    | 2.30                     | 0.46              |
| 35:BA:2572:A:N7    | 39:BE:144:ARG:HD2  | 2.30                     | 0.46              |
| 35:BA:2581:G:C6    | 35:BA:2610:C:C2    | 3.02                     | 0.46              |
| 35:BA:2741:A:H2'   | 35:BA:2742:C:O4'   | 2.15                     | 0.46              |
| 35:BA:361:G:C2'    | 35:BA:362:U:H5''   | 2.38                     | 0.46              |
| 35:BA:843:G:C2'    | 35:BA:844:C:H5'    | 2.45                     | 0.46              |
| 36:BB:22:U:H2'     | 36:BB:23:G:H8      | 1.79                     | 0.46              |
| 36:BB:50:G:OP2     | 51:BS:62:LYS:HD3   | 2.15                     | 0.46              |
| 36:BB:5:C:O2'      | 36:BB:6:C:H5'      | 2.14                     | 0.46              |
| 36:BB:67:G:O2'     | 36:BB:68:C:H6      | 1.97                     | 0.46              |
| 37:BC:108:TRP:CD1  | 37:BC:108:TRP:N    | 2.82                     | 0.46              |
| 37:BC:115:VAL:HG22 | 37:BC:150:ILE:HD13 | 1.97                     | 0.46              |
| 37:BC:54:ARG:HH22  | 37:BC:56:ASP:HB3   | 1.76                     | 0.46              |
| 37:BC:68:GLY:N     | 37:BC:189:ASN:ND2  | 2.62                     | 0.46              |
| 40:BF:122:LYS:HG3  | 40:BF:191:ARG:HA   | 1.97                     | 0.46              |
| 40:BF:63:LYS:NZ    | 40:BF:75:HIS:O     | 2.48                     | 0.46              |
| 43:BJ:109:UNK:C    | 43:BJ:111:UNK:N    | 2.78                     | 0.46              |
| 50:BR:9:LYS:HG3    | 50:BR:43:GLU:OE1   | 2.15                     | 0.46              |
| 51:BS:54:LEU:C     | 51:BS:56:LEU:N     | 2.68                     | 0.46              |
| 51:BS:95:HIS:CG    | 51:BS:96:GLY:N     | 2.84                     | 0.46              |
| 52:BT:16:ARG:NH1   | 52:BT:18:ASP:OD1   | 2.49                     | 0.46              |
| 1:AA:135:C:H2'     | 1:AA:136:C:H5'     | 1.97                     | 0.46              |
| 1:AA:1407:C:H2'    | 1:AA:1408:A:H5'    | 1.97                     | 0.46              |
| 1:AA:545:C:O2'     | 1:AA:546:G:C5'     | 2.63                     | 0.46              |
| 1:AA:559:A:H1'     | 1:AA:561:U:O2'     | 2.16                     | 0.46              |
| 1:AA:589:C:C2'     | 1:AA:590:C:H5'     | 2.44                     | 0.46              |
| 1:AA:688:G:C2'     | 1:AA:689:C:C5'     | 2.93                     | 0.46              |
| 2:AB:21:ARG:C      | 2:AB:23:ARG:H      | 2.16                     | 0.46              |
| 3:AC:115:LEU:O     | 3:AC:118:GLN:HB3   | 2.15                     | 0.46              |
| 3:AC:50:ALA:HB2    | 3:AC:75:VAL:HG11   | 1.93                     | 0.46              |
| 3:AC:74:GLY:O      | 3:AC:78:GLY:CA     | 2.64                     | 0.46              |
| 4:AD:36:ARG:C      | 4:AD:38:TYR:H      | 2.19                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:5:ILE:O       | 4:AD:5:ILE:HG22    | 2.15                     | 0.46              |
| 16:AP:8:ARG:NH2    | 16:AP:15:PRO:HG3   | 2.30                     | 0.46              |
| 19:AS:42:PRO:HG2   | 19:AS:43:GLU:H     | 1.80                     | 0.46              |
| 24:AY:241:GLU:O    | 24:AY:245:ALA:HB2  | 2.16                     | 0.46              |
| 24:AY:455:GLY:O    | 24:AY:458:HIS:HB3  | 2.15                     | 0.46              |
| 27:B2:5:GLU:O      | 27:B2:9:GLN:OE1    | 2.33                     | 0.46              |
| 31:B6:53:LYS:CG    | 31:B6:54:ILE:N     | 2.78                     | 0.46              |
| 33:B8:60:LEU:O     | 33:B8:63:PRO:HG2   | 2.15                     | 0.46              |
| 35:BA:1353:A:C8    | 35:BA:1378:A:N6    | 2.83                     | 0.46              |
| 35:BA:1431:U:H2'   | 35:BA:1432:C:C6    | 2.50                     | 0.46              |
| 35:BA:1599:C:H2'   | 35:BA:1600:C:H6    | 1.81                     | 0.46              |
| 35:BA:1773:A:C8    | 35:BA:1829:A:C8    | 3.03                     | 0.46              |
| 35:BA:1797:C:C2'   | 35:BA:1798:U:H5'   | 2.45                     | 0.46              |
| 35:BA:18:C:H6      | 35:BA:18:C:O5'     | 1.99                     | 0.46              |
| 35:BA:1988:C:H2'   | 35:BA:1989:G:H8    | 1.80                     | 0.46              |
| 35:BA:2200:C:H42   | 35:BA:2223:G:H1    | 1.62                     | 0.46              |
| 35:BA:2714:G:C6    | 35:BA:2715:C:C4    | 3.03                     | 0.46              |
| 35:BA:271(E):U:H2' | 35:BA:271(F):C:C6  | 2.51                     | 0.46              |
| 32:B7:33:ARG:NH1   | 35:BA:467:G:OP1    | 2.47                     | 0.46              |
| 35:BA:833:U:H5'    | 48:BP:51:PHE:O     | 2.11                     | 0.46              |
| 39:BE:98:PRO:HG3   | 39:BE:175:VAL:HG12 | 1.97                     | 0.46              |
| 36:BB:43:C:C4'     | 41:BG:94:LEU:HD11  | 2.44                     | 0.46              |
| 46:BN:133:GLN:C    | 46:BN:134:ARG:HG2  | 2.36                     | 0.46              |
| 46:BN:39:ARG:HE    | 46:BN:41:ASP:HB2   | 1.80                     | 0.46              |
| 52:BT:109:GLU:HG2  | 52:BT:112:ARG:CZ   | 2.45                     | 0.46              |
| 52:BT:3:ARG:O      | 52:BT:4:GLY:C      | 2.53                     | 0.46              |
| 53:BU:90:VAL:CG1   | 54:BV:39:LEU:HG    | 2.29                     | 0.46              |
| 54:BV:47:VAL:C     | 54:BV:49:THR:H     | 2.17                     | 0.46              |
| 1:AA:1452:C:OP2    | 1:AA:1457:G:C6     | 2.69                     | 0.46              |
| 1:AA:266:G:C4'     | 1:AA:267:C:C6      | 2.99                     | 0.46              |
| 1:AA:309:G:H2'     | 1:AA:310:G:H8      | 1.80                     | 0.46              |
| 1:AA:61:G:C2'      | 1:AA:62:U:H5'      | 2.46                     | 0.46              |
| 1:AA:84:U:O2       | 1:AA:84:U:O4'      | 2.32                     | 0.46              |
| 1:AA:859:A:H2'     | 1:AA:860:A:H8      | 1.81                     | 0.46              |
| 1:AA:869:G:O5'     | 1:AA:869:G:H8      | 1.97                     | 0.46              |
| 1:AA:942:G:C2      | 1:AA:943:U:C6      | 3.03                     | 0.46              |
| 2:AB:16:HIS:ND1    | 2:AB:210:SER:HA    | 2.30                     | 0.46              |
| 2:AB:227:GLY:O     | 2:AB:228:GLY:C     | 2.54                     | 0.46              |
| 1:AA:972:C:O3'     | 10:AJ:57:LYS:HG2   | 2.16                     | 0.46              |
| 24:AY:238:THR:C    | 24:AY:240:GLU:H    | 2.18                     | 0.46              |
| 24:AY:49:ALA:N     | 24:AY:52:MET:HB3   | 2.31                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:B2:47:ASN:C    | 27:B2:49:LYS:N     | 2.67                     | 0.46              |
| 35:BA:1336:A:H2'  | 35:BA:1337:G:C8    | 2.49                     | 0.46              |
| 35:BA:157:U:O2'   | 35:BA:158:U:H5'    | 2.15                     | 0.46              |
| 35:BA:1828:G:O6   | 38:BD:222:ARG:HD2  | 2.16                     | 0.46              |
| 35:BA:2650:U:H2'  | 35:BA:2651:C:C6    | 2.50                     | 0.46              |
| 35:BA:2716:U:O2'  | 35:BA:2717:G:C5'   | 2.48                     | 0.46              |
| 37:BC:126:SER:C   | 37:BC:128:LEU:H    | 2.19                     | 0.46              |
| 38:BD:108:PRO:HB3 | 38:BD:143:HIS:HE1  | 1.79                     | 0.46              |
| 38:BD:164:GLN:O   | 38:BD:166:GLN:NE2  | 2.48                     | 0.46              |
| 39:BE:55:ASN:O    | 39:BE:56:PRO:O     | 2.34                     | 0.46              |
| 39:BE:76:ARG:CG   | 39:BE:195:LEU:HD22 | 2.42                     | 0.46              |
| 41:BG:29:TRP:O    | 41:BG:31:VAL:N     | 2.46                     | 0.46              |
| 46:BN:134:ARG:H   | 46:BN:135:PRO:HD3  | 1.80                     | 0.46              |
| 47:BO:102:VAL:HB  | 47:BO:106:LEU:HD12 | 1.98                     | 0.46              |
| 56:BX:27:THR:HA   | 56:BX:80:ILE:HA    | 1.97                     | 0.46              |
| 57:BY:89:PHE:O    | 57:BY:90:LEU:HD23  | 2.16                     | 0.46              |
| 49:BQ:134:ARG:CZ  | 58:BZ:122:ARG:NH2  | 2.79                     | 0.46              |
| 58:BZ:181:GLU:C   | 58:BZ:182:LYS:HG3  | 2.35                     | 0.46              |
| 58:BZ:5:LEU:HD23  | 58:BZ:47:VAL:CG2   | 2.30                     | 0.46              |
| 58:BZ:77:ASP:O    | 58:BZ:78:LYS:HB2   | 2.16                     | 0.46              |
| 1:AA:1157:A:C4    | 1:AA:1181:G:C2     | 3.04                     | 0.46              |
| 1:AA:346:G:O2'    | 1:AA:347:G:OP2     | 2.33                     | 0.46              |
| 1:AA:38:G:O2'     | 1:AA:39:G:O5'      | 2.30                     | 0.46              |
| 1:AA:77:G:H1      | 1:AA:92:C:H42      | 1.63                     | 0.46              |
| 3:AC:14:ILE:CG1   | 3:AC:15:THR:N      | 2.79                     | 0.46              |
| 3:AC:10:PHE:CZ    | 3:AC:178:LEU:HD11  | 2.51                     | 0.46              |
| 7:AG:120:ILE:O    | 7:AG:121:ALA:CB    | 2.59                     | 0.46              |
| 7:AG:22:LEU:O     | 7:AG:23:VAL:HB     | 2.15                     | 0.46              |
| 12:AL:17:LYS:CD   | 12:AL:18:VAL:N     | 2.76                     | 0.46              |
| 17:AQ:59:ILE:HG23 | 17:AQ:71:PHE:HB3   | 1.98                     | 0.46              |
| 24:AY:296:GLY:O   | 24:AY:297:GLU:HB3  | 2.14                     | 0.46              |
| 25:B0:51:VAL:CA   | 25:B0:62:LEU:HD21  | 2.45                     | 0.46              |
| 26:B1:11:ARG:NH2  | 35:BA:1365:A:O2'   | 2.49                     | 0.46              |
| 27:B2:9:GLN:C     | 27:B2:11:GLU:N     | 2.69                     | 0.46              |
| 35:BA:1063:G:H1   | 35:BA:1074:G:H1    | 1.63                     | 0.46              |
| 35:BA:1133:U:HO3' | 35:BA:1135:C:P     | 2.38                     | 0.46              |
| 35:BA:1265:A:H8   | 35:BA:1265:A:OP1   | 1.99                     | 0.46              |
| 35:BA:1285:G:H8   | 35:BA:1285:G:O5'   | 1.99                     | 0.46              |
| 35:BA:1591:G:H8   | 35:BA:1591:G:H5'   | 1.80                     | 0.46              |
| 35:BA:1639:U:H2'  | 35:BA:1640:C:C5'   | 2.46                     | 0.46              |
| 35:BA:1993:U:H2'  | 35:BA:1994:C:H6    | 1.80                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2748:A:C4    | 35:BA:2757:A:N6    | 2.83                     | 0.46              |
| 35:BA:832:G:P      | 48:BP:40:SER:HB3   | 2.55                     | 0.46              |
| 36:BB:37:C:C2'     | 36:BB:38:C:H5'     | 2.45                     | 0.46              |
| 37:BC:117:THR:CG2  | 37:BC:119:ASP:CG   | 2.81                     | 0.46              |
| 37:BC:123:ALA:O    | 37:BC:127:LYS:CG   | 2.63                     | 0.46              |
| 37:BC:223:VAL:O    | 37:BC:223:VAL:HG23 | 2.15                     | 0.46              |
| 37:BC:88:GLU:CG    | 37:BC:89:GLU:H     | 2.18                     | 0.46              |
| 38:BD:124:PRO:O    | 38:BD:126:GLN:HG2  | 2.16                     | 0.46              |
| 39:BE:111:ARG:C    | 50:BR:2:ARG:HG2    | 2.36                     | 0.46              |
| 39:BE:19:ARG:HA    | 47:BO:73:ASP:HA    | 1.96                     | 0.46              |
| 40:BF:4:VAL:N      | 40:BF:24:LEU:HD12  | 2.30                     | 0.46              |
| 41:BG:118:ARG:HH12 | 41:BG:182:LYS:HD3  | 1.79                     | 0.46              |
| 41:BG:16:ARG:O     | 41:BG:20:ILE:HG13  | 2.16                     | 0.46              |
| 41:BG:32:PRO:HB3   | 41:BG:163:ALA:HB2  | 1.96                     | 0.46              |
| 41:BG:57:ALA:O     | 41:BG:61:ALA:CB    | 2.63                     | 0.46              |
| 41:BG:61:ALA:CB    | 41:BG:67:LYS:HA    | 2.42                     | 0.46              |
| 42:BH:168:PRO:CB   | 42:BH:170:ARG:NH2  | 2.78                     | 0.46              |
| 42:BH:30:LYS:HZ3   | 42:BH:80:SER:HA    | 1.80                     | 0.46              |
| 44:BK:76:UNK:C     | 44:BK:78:UNK:N     | 2.75                     | 0.46              |
| 47:BO:36:GLY:HA3   | 47:BO:109:LYS:HD2  | 1.96                     | 0.46              |
| 35:BA:2723:C:O3'   | 50:BR:2:ARG:NH2    | 2.49                     | 0.46              |
| 50:BR:57:ARG:HB3   | 50:BR:59:ASP:OD1   | 2.15                     | 0.46              |
| 51:BS:28:VAL:CG1   | 51:BS:29:PHE:N     | 2.76                     | 0.46              |
| 46:BN:40:PRO:HB3   | 53:BU:68:ALA:HB2   | 1.97                     | 0.46              |
| 58:BZ:114:GLY:C    | 58:BZ:177:PRO:HD3  | 2.36                     | 0.46              |
| 1:AA:1279:A:H5''   | 1:AA:1280:A:P      | 2.55                     | 0.46              |
| 1:AA:366:C:O5'     | 1:AA:366:C:H6      | 1.98                     | 0.46              |
| 1:AA:827:U:H3      | 1:AA:872:A:H61     | 1.62                     | 0.46              |
| 1:AA:930:C:O2'     | 1:AA:931:C:H5'     | 2.15                     | 0.46              |
| 1:AA:946:A:N1      | 1:AA:947:G:C6      | 2.83                     | 0.46              |
| 1:AA:958:A:H8      | 1:AA:958:A:O5'     | 1.99                     | 0.46              |
| 2:AB:90:MET:HB3    | 2:AB:91:PRO:HD2    | 1.97                     | 0.46              |
| 3:AC:191:THR:CG2   | 3:AC:192:THR:N     | 2.79                     | 0.46              |
| 10:AJ:28:ARG:NH1   | 10:AJ:34:VAL:HB    | 2.31                     | 0.46              |
| 16:AP:60:LEU:HD21  | 16:AP:66:PRO:CG    | 2.44                     | 0.46              |
| 24:AY:357:ARG:NH1  | 24:AY:357:ARG:HG3  | 2.31                     | 0.46              |
| 24:AY:324:ARG:HD3  | 24:AY:380:LEU:O    | 2.15                     | 0.46              |
| 26:B1:59:THR:O     | 26:B1:60:PHE:CG    | 2.67                     | 0.46              |
| 28:B3:54:VAL:O     | 28:B3:54:VAL:CG2   | 2.63                     | 0.46              |
| 35:BA:1240:U:O2'   | 35:BA:1241:A:H5'   | 2.16                     | 0.46              |
| 35:BA:1478:G:HO2'  | 35:BA:1558:A:H2    | 1.61                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:1689:A:H62   | 35:BA:1698:A:H2   | 1.63                     | 0.46              |
| 35:BA:2125:G:O5'   | 35:BA:2125:G:H8   | 1.99                     | 0.46              |
| 35:BA:2317:C:O2'   | 35:BA:2318:G:H5'  | 2.15                     | 0.46              |
| 35:BA:2287:A:H2    | 35:BA:2346:A:N1   | 2.14                     | 0.46              |
| 35:BA:2533:A:OP1   | 35:BA:2665:A:H1'  | 2.15                     | 0.46              |
| 35:BA:2770:G:C5'   | 35:BA:2771:C:OP2  | 2.64                     | 0.46              |
| 35:BA:34:C:N4      | 35:BA:447:A:N6    | 2.63                     | 0.46              |
| 35:BA:602:G:N1     | 35:BA:654(U):A:N7 | 2.64                     | 0.46              |
| 35:BA:904:C:O2'    | 35:BA:905:U:H5'   | 2.15                     | 0.46              |
| 37:BC:46:ALA:O     | 37:BC:47:LYS:HB2  | 2.15                     | 0.46              |
| 39:BE:132:HIS:CA   | 39:BE:135:HIS:NE2 | 2.79                     | 0.46              |
| 35:BA:2572:A:C8    | 39:BE:144:ARG:HD2 | 2.50                     | 0.46              |
| 35:BA:574:C:N3     | 39:BE:145:LYS:HE2 | 2.31                     | 0.46              |
| 39:BE:57:LYS:HA    | 39:BE:57:LYS:CE   | 2.27                     | 0.46              |
| 40:BF:125:LEU:HD23 | 40:BF:125:LEU:N   | 2.29                     | 0.46              |
| 40:BF:22:ALA:HB1   | 40:BF:26:ALA:HB2  | 1.97                     | 0.46              |
| 41:BG:42:GLY:O     | 41:BG:47:LYS:HD2  | 2.15                     | 0.46              |
| 42:BH:85:LYS:HZ3   | 42:BH:87:LEU:CG   | 2.27                     | 0.46              |
| 44:BK:10:UNK:O     | 44:BK:11:UNK:CB   | 2.63                     | 0.46              |
| 45:BL:115:UNK:O    | 45:BL:116:UNK:C   | 2.63                     | 0.46              |
| 45:BL:65:UNK:O     | 45:BL:67:UNK:N    | 2.49                     | 0.46              |
| 50:BR:2:ARG:CG     | 50:BR:2:ARG:NH1   | 2.71                     | 0.46              |
| 51:BS:30:ARG:HD3   | 51:BS:97:ARG:CG   | 2.34                     | 0.46              |
| 52:BT:10:VAL:O     | 52:BT:13:ARG:HG2  | 2.14                     | 0.46              |
| 58:BZ:149:SER:HB2  | 58:BZ:173:ALA:CA  | 2.39                     | 0.46              |
| 1:AA:1037:C:C2     | 1:AA:1038:C:N3    | 2.84                     | 0.46              |
| 1:AA:1151:A:O4'    | 10:AJ:39:PRO:HB2  | 2.16                     | 0.46              |
| 1:AA:1286:A:HO2'   | 1:AA:1287:A:H5''  | 1.80                     | 0.46              |
| 1:AA:1250:A:H2     | 1:AA:1370:G:H1'   | 1.81                     | 0.46              |
| 1:AA:555:C:N4      | 1:AA:556:C:H42    | 2.12                     | 0.46              |
| 1:AA:557:G:O2'     | 1:AA:558:G:H5'    | 2.16                     | 0.46              |
| 1:AA:602:A:H2'     | 1:AA:603:U:C6     | 2.51                     | 0.46              |
| 1:AA:614:A:O2'     | 1:AA:615:C:H5'    | 2.16                     | 0.46              |
| 1:AA:701:C:H6      | 1:AA:701:C:H3'    | 1.80                     | 0.46              |
| 1:AA:841:U:H3'     | 1:AA:848:C:O4'    | 2.15                     | 0.46              |
| 2:AB:76:GLN:HE21   | 2:AB:76:GLN:H     | 1.63                     | 0.46              |
| 3:AC:11:ARG:O      | 3:AC:14:ILE:O     | 2.34                     | 0.46              |
| 3:AC:60:ALA:O      | 3:AC:62:ASP:N     | 2.45                     | 0.46              |
| 7:AG:88:PRO:O      | 7:AG:89:MET:HB3   | 2.15                     | 0.46              |
| 24:AY:628:ARG:NH1  | 24:AY:628:ARG:CG  | 2.76                     | 0.46              |
| 25:B0:25:ARG:CB    | 25:B0:37:LEU:HD12 | 2.43                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:B2:9:GLN:NE2    | 27:B2:9:GLN:H      | 2.08                     | 0.46              |
| 32:B7:34:ARG:HB2   | 32:B7:42:LEU:HD22  | 1.96                     | 0.46              |
| 35:BA:1639:U:H6    | 35:BA:1639:U:O5'   | 1.99                     | 0.46              |
| 35:BA:1983:C:O2'   | 35:BA:1984:G:H5'   | 1.99                     | 0.46              |
| 35:BA:2126:A:HO2'  | 35:BA:2127:G:H8    | 1.63                     | 0.46              |
| 35:BA:2203:U:C3'   | 35:BA:2205:C:OP2   | 2.64                     | 0.46              |
| 35:BA:535:C:C2'    | 35:BA:536:A:H5'    | 2.46                     | 0.46              |
| 35:BA:742:G:C2'    | 35:BA:743:G:H5''   | 2.22                     | 0.46              |
| 35:BA:999:U:O2'    | 35:BA:1000:A:H5'   | 2.16                     | 0.46              |
| 37:BC:30:VAL:CG2   | 37:BC:31:LYS:H     | 2.27                     | 0.46              |
| 38:BD:27:THR:CG2   | 38:BD:83:GLU:CG    | 2.90                     | 0.46              |
| 39:BE:38:THR:HG22  | 39:BE:40:GLU:H     | 1.81                     | 0.46              |
| 39:BE:65:GLY:C     | 39:BE:67:PHE:N     | 2.69                     | 0.46              |
| 41:BG:144:ILE:HD11 | 41:BG:146:TYR:CE1  | 2.50                     | 0.46              |
| 41:BG:162:THR:O    | 41:BG:163:ALA:O    | 2.34                     | 0.46              |
| 42:BH:149:ARG:HA   | 42:BH:162:ILE:HD11 | 1.94                     | 0.46              |
| 48:BP:105:LEU:O    | 48:BP:106:LEU:HB3  | 2.16                     | 0.46              |
| 35:BA:812:C:H5'    | 48:BP:25:SER:CB    | 2.45                     | 0.46              |
| 48:BP:48:PRO:HB2   | 48:BP:51:PHE:O     | 2.15                     | 0.46              |
| 50:BR:44:LEU:HD13  | 50:BR:44:LEU:O     | 2.16                     | 0.46              |
| 50:BR:97:VAL:C     | 50:BR:98:LEU:HD23  | 2.35                     | 0.46              |
| 52:BT:134:GLU:O    | 52:BT:135:ALA:HB3  | 2.16                     | 0.46              |
| 52:BT:78:LEU:HB3   | 52:BT:79:HIS:CD2   | 2.51                     | 0.46              |
| 35:BA:2849:U:OP2   | 52:BT:95:ARG:NH1   | 2.49                     | 0.46              |
| 57:BY:10:GLY:CA    | 57:BY:27:VAL:HG12  | 2.46                     | 0.46              |
| 57:BY:50:ARG:NE    | 57:BY:55:TYR:O     | 2.48                     | 0.46              |
| 58:BZ:151:HIS:CG   | 58:BZ:170:THR:HA   | 2.51                     | 0.46              |
| 1:AA:1408:A:H5'    | 1:AA:1408:A:C8     | 2.43                     | 0.46              |
| 1:AA:892:A:O2'     | 1:AA:1415:G:H4'    | 2.15                     | 0.46              |
| 1:AA:1405:G:O4'    | 1:AA:1519:A:H4'    | 2.16                     | 0.46              |
| 1:AA:185:A:C4      | 1:AA:186:C:C5      | 3.03                     | 0.46              |
| 1:AA:364:A:H8      | 1:AA:364:A:O5'     | 1.99                     | 0.46              |
| 1:AA:599:C:O2'     | 1:AA:600:C:H5'     | 2.16                     | 0.46              |
| 1:AA:648:A:H2'     | 1:AA:649:G:H8      | 1.81                     | 0.46              |
| 1:AA:982:U:O2'     | 1:AA:983:A:OP2     | 2.30                     | 0.46              |
| 3:AC:21:ARG:O      | 3:AC:22:TRP:HB3    | 2.15                     | 0.46              |
| 6:AF:86:ARG:O      | 6:AF:87:ARG:HB2    | 2.16                     | 0.46              |
| 18:AR:53:ARG:C     | 18:AR:55:ARG:N     | 2.69                     | 0.46              |
| 18:AR:53:ARG:O     | 18:AR:55:ARG:N     | 2.49                     | 0.46              |
| 24:AY:246:ILE:HG23 | 24:AY:255:ILE:CD1  | 2.46                     | 0.46              |
| 24:AY:448:GLN:OE1  | 24:AY:480:GLN:HG3  | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:445:GLU:OE1  | 24:AY:482:ALA:HB1  | 2.16                     | 0.46              |
| 26:B1:5:CYS:SG     | 26:B1:8:SER:CB     | 3.04                     | 0.46              |
| 29:B4:21:VAL:HG12  | 29:B4:22:ILE:HD13  | 1.97                     | 0.46              |
| 30:B5:40:LYS:HE2   | 30:B5:46:CYS:CB    | 2.43                     | 0.46              |
| 30:B5:57:VAL:HG12  | 30:B5:58:LEU:CD1   | 2.46                     | 0.46              |
| 31:B6:11:LEU:C     | 31:B6:11:LEU:CD2   | 2.83                     | 0.46              |
| 33:B8:50:LEU:C     | 33:B8:52:LYS:N     | 2.68                     | 0.46              |
| 35:BA:1142(A):A:N3 | 35:BA:1144:G:C8    | 2.84                     | 0.46              |
| 35:BA:1820:U:O2'   | 35:BA:1821:A:OP1   | 2.30                     | 0.46              |
| 35:BA:604:G:C2'    | 35:BA:605:C:C5'    | 2.77                     | 0.46              |
| 36:BB:42:C:O2'     | 36:BB:43:C:P       | 2.74                     | 0.46              |
| 38:BD:181:GLU:HB2  | 38:BD:273:ARG:O    | 2.16                     | 0.46              |
| 40:BF:125:LEU:HD12 | 40:BF:196:LEU:HD23 | 1.98                     | 0.46              |
| 35:BA:2751:G:C6    | 42:BH:1:MET:CG     | 2.99                     | 0.46              |
| 45:BL:83:UNK:O     | 45:BL:86:UNK:CB    | 2.64                     | 0.46              |
| 46:BN:132:ALA:O    | 46:BN:133:GLN:HB3  | 2.15                     | 0.46              |
| 46:BN:1:MET:SD     | 46:BN:1:MET:C      | 2.94                     | 0.46              |
| 46:BN:39:ARG:HH21  | 46:BN:41:ASP:CG    | 2.19                     | 0.46              |
| 48:BP:91:PHE:CD1   | 48:BP:91:PHE:N     | 2.84                     | 0.46              |
| 52:BT:7:ILE:O      | 52:BT:11:GLU:OE1   | 2.34                     | 0.46              |
| 54:BV:55:ALA:HA    | 54:BV:100:ARG:O    | 2.15                     | 0.46              |
| 55:BW:75:TYR:O     | 55:BW:104:THR:HG23 | 2.15                     | 0.46              |
| 1:AA:769:G:H4'     | 1:AA:1513:A:H4'    | 1.98                     | 0.46              |
| 1:AA:66:G:H4'      | 1:AA:173:U:C5      | 2.51                     | 0.46              |
| 1:AA:185:A:H2'     | 1:AA:186:C:C6      | 2.50                     | 0.46              |
| 1:AA:307:C:C5      | 1:AA:308:C:N4      | 2.84                     | 0.46              |
| 1:AA:492:G:H2'     | 1:AA:493:G:O5'     | 2.14                     | 0.46              |
| 1:AA:547:A:C1'     | 1:AA:548:G:P       | 3.03                     | 0.46              |
| 1:AA:863:U:O2      | 1:AA:863:U:H3'     | 2.16                     | 0.46              |
| 1:AA:925:G:N3      | 1:AA:1502:A:H1'    | 2.31                     | 0.46              |
| 3:AC:11:ARG:CG     | 3:AC:11:ARG:HH11   | 2.28                     | 0.46              |
| 3:AC:148:GLY:HA3   | 3:AC:172:ARG:O     | 2.16                     | 0.46              |
| 4:AD:109:GLY:O     | 4:AD:111:ALA:N     | 2.49                     | 0.46              |
| 6:AF:79:LEU:O      | 6:AF:85:VAL:HG11   | 2.15                     | 0.46              |
| 8:AH:84:ARG:NH2    | 8:AH:136:GLU:OE2   | 2.49                     | 0.46              |
| 9:AI:4:TYR:CG      | 9:AI:88:TYR:HB2    | 2.50                     | 0.46              |
| 11:AK:40:ILE:HG23  | 11:AK:75:TYR:CE2   | 2.51                     | 0.46              |
| 24:AY:487:ILE:N    | 24:AY:487:ILE:HD13 | 2.28                     | 0.46              |
| 24:AY:616:TYR:CD2  | 24:AY:663:THR:HA   | 2.51                     | 0.46              |
| 25:B0:39:ARG:HG3   | 25:B0:39:ARG:O     | 2.15                     | 0.46              |
| 28:B3:3:ARG:HA     | 28:B3:37:LEU:O     | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:B9:7:VAL:HG13   | 34:B9:25:VAL:HG23  | 1.98                     | 0.46              |
| 35:BA:1027:A:H61   | 35:BA:1126:A:C1'   | 2.29                     | 0.46              |
| 35:BA:1187:G:H5''  | 54:BV:81:TYR:HE2   | 1.73                     | 0.46              |
| 35:BA:1434:A:O2'   | 35:BA:1435:G:H5'   | 2.16                     | 0.46              |
| 35:BA:1528:A:C2    | 35:BA:1542:A:H2    | 2.34                     | 0.46              |
| 35:BA:1982:C:C2    | 35:BA:1983:C:C5    | 3.04                     | 0.46              |
| 35:BA:2403:C:C2    | 35:BA:2404:C:C5    | 3.03                     | 0.46              |
| 35:BA:267:C:C2     | 35:BA:268:C:C5     | 3.04                     | 0.46              |
| 35:BA:1297:C:OP1   | 35:BA:2710:C:H4'   | 2.16                     | 0.46              |
| 35:BA:2715:C:C2'   | 35:BA:2716:U:C5'   | 2.90                     | 0.46              |
| 35:BA:2791:C:H4'   | 35:BA:2792:G:O5'   | 2.14                     | 0.46              |
| 35:BA:332:A:C5     | 35:BA:335:C:N4     | 2.83                     | 0.46              |
| 35:BA:863:A:O2'    | 35:BA:864:G:H5'    | 2.16                     | 0.46              |
| 36:BB:50:G:OP1     | 51:BS:63:THR:HG23  | 2.15                     | 0.46              |
| 37:BC:20:VAL:O     | 37:BC:224:ARG:O    | 2.34                     | 0.46              |
| 39:BE:46:ALA:HB2   | 39:BE:82:ARG:HA    | 1.97                     | 0.46              |
| 35:BA:590:A:OP1    | 40:BF:95:ARG:NH1   | 2.49                     | 0.46              |
| 41:BG:6:ALA:O      | 41:BG:7:LEU:C      | 2.52                     | 0.46              |
| 41:BG:7:LEU:HD11   | 41:BG:176:LEU:CD2  | 2.46                     | 0.46              |
| 42:BH:154:PRO:HB2  | 42:BH:163:TYR:CZ   | 2.50                     | 0.46              |
| 47:BO:86:ILE:HG22  | 47:BO:94:ARG:HG3   | 1.98                     | 0.46              |
| 48:BP:98:GLU:HA    | 48:BP:101:VAL:HG22 | 1.98                     | 0.46              |
| 49:BQ:109:VAL:HG12 | 49:BQ:113:GLN:OE1  | 2.15                     | 0.46              |
| 52:BT:34:VAL:HG13  | 52:BT:39:ARG:CA    | 2.45                     | 0.46              |
| 52:BT:88:ILE:HG22  | 52:BT:89:VAL:N     | 2.30                     | 0.46              |
| 1:AA:1068:G:N7     | 1:AA:1094:G:H2'    | 2.30                     | 0.46              |
| 1:AA:1250:A:C2     | 1:AA:1370:G:H1'    | 2.50                     | 0.46              |
| 1:AA:551:U:H2'     | 1:AA:552:U:C6      | 2.51                     | 0.46              |
| 1:AA:90:U:C4'      | 1:AA:91:C:OP1      | 2.64                     | 0.46              |
| 4:AD:60:GLU:HG2    | 4:AD:202:LEU:HD12  | 1.98                     | 0.46              |
| 8:AH:132:GLU:HG2   | 8:AH:134:ILE:HD13  | 1.96                     | 0.46              |
| 11:AK:115:PRO:C    | 11:AK:117:ASN:H    | 2.19                     | 0.46              |
| 11:AK:65:ALA:O     | 11:AK:68:ALA:HB3   | 2.15                     | 0.46              |
| 1:AA:192:U:H1'     | 20:AT:103:GLY:HA2  | 1.97                     | 0.46              |
| 1:AA:1494:G:O3'    | 24:AY:499:ARG:NH2  | 2.49                     | 0.46              |
| 25:B0:66:VAL:CG1   | 25:B0:67:VAL:H     | 2.28                     | 0.46              |
| 31:B6:26:ASN:O     | 31:B6:27:LYS:HB2   | 2.15                     | 0.46              |
| 33:B8:4:MET:HB3    | 33:B8:61:LEU:CD2   | 2.45                     | 0.46              |
| 35:BA:185:U:H2'    | 35:BA:186:G:C8     | 2.51                     | 0.46              |
| 35:BA:2208:A:H1'   | 35:BA:2219:G:C6    | 2.51                     | 0.46              |
| 25:B0:16:SER:HB2   | 35:BA:2262:U:C5    | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:363(A):A:N3  | 35:BA:363(A):A:H2' | 2.31                     | 0.46              |
| 35:BA:426:C:O2'    | 35:BA:427:U:H5'    | 2.16                     | 0.46              |
| 35:BA:34:C:H42     | 35:BA:447:A:N6     | 2.13                     | 0.46              |
| 35:BA:686:G:H21    | 35:BA:788:A:H61    | 1.64                     | 0.46              |
| 35:BA:831:G:O3'    | 48:BP:40:SER:HB3   | 2.16                     | 0.46              |
| 36:BB:64:C:H2'     | 36:BB:65:C:C6      | 2.51                     | 0.46              |
| 40:BF:65:TRP:CZ3   | 40:BF:73:ALA:O     | 2.69                     | 0.46              |
| 41:BG:43:LEU:HD13  | 41:BG:53:LEU:HD12  | 1.97                     | 0.46              |
| 41:BG:87:PRO:O     | 41:BG:88:ILE:HB    | 2.16                     | 0.46              |
| 42:BH:126:PRO:HG2  | 42:BH:127:GLU:H    | 1.81                     | 0.46              |
| 42:BH:19:VAL:HG12  | 42:BH:20:ALA:N     | 2.31                     | 0.46              |
| 47:BO:114:ILE:HD12 | 47:BO:114:ILE:H    | 1.81                     | 0.46              |
| 48:BP:61:ARG:C     | 48:BP:62:LEU:CD2   | 2.84                     | 0.46              |
| 48:BP:84:ASN:ND2   | 48:BP:115:LEU:HD23 | 2.30                     | 0.46              |
| 49:BQ:104:PHE:O    | 49:BQ:105:GLU:HB3  | 2.15                     | 0.46              |
| 1:AA:1145:C:O2'    | 1:AA:1146:A:O5'    | 2.32                     | 0.45              |
| 1:AA:1286:A:O2'    | 1:AA:1287:A:OP2    | 2.30                     | 0.45              |
| 1:AA:1305:G:C6     | 1:AA:1331:G:C6     | 3.05                     | 0.45              |
| 1:AA:644:G:H5'     | 8:AH:92:ARG:NH2    | 2.31                     | 0.45              |
| 1:AA:769:G:O2'     | 1:AA:770:C:C5'     | 2.62                     | 0.45              |
| 1:AA:791:G:O5'     | 1:AA:791:G:H8      | 1.98                     | 0.45              |
| 3:AC:16:ARG:CG     | 3:AC:17:ASP:N      | 2.79                     | 0.45              |
| 4:AD:15:GLU:C      | 4:AD:17:VAL:H      | 2.18                     | 0.45              |
| 5:AE:33:VAL:HG11   | 5:AE:109:ILE:HA    | 1.98                     | 0.45              |
| 8:AH:86:ILE:HB     | 8:AH:133:LEU:O     | 2.16                     | 0.45              |
| 8:AH:8:ASP:O       | 8:AH:12:ARG:HG3    | 2.15                     | 0.45              |
| 9:AI:40:LEU:O      | 9:AI:42:ARG:N      | 2.49                     | 0.45              |
| 9:AI:8:GLY:HA2     | 9:AI:79:LEU:HD12   | 1.97                     | 0.45              |
| 9:AI:99:LEU:N      | 9:AI:99:LEU:HD22   | 2.30                     | 0.45              |
| 12:AL:123:LYS:N    | 12:AL:123:LYS:CE   | 2.78                     | 0.45              |
| 24:AY:548:GLU:C    | 24:AY:550:MET:H    | 2.18                     | 0.45              |
| 24:AY:526:VAL:HG11 | 24:AY:566:THR:HG23 | 1.96                     | 0.45              |
| 26:B1:67:ILE:N     | 26:B1:68:PRO:HD2   | 2.31                     | 0.45              |
| 27:B2:10:LEU:HB3   | 27:B2:14:ARG:NH1   | 2.31                     | 0.45              |
| 27:B2:50:ILE:HG21  | 35:BA:61:G:H5'     | 1.98                     | 0.45              |
| 29:B4:40:HIS:NE2   | 41:BG:118:ARG:CA   | 2.74                     | 0.45              |
| 31:B6:53:LYS:O     | 31:B6:54:ILE:C     | 2.54                     | 0.45              |
| 35:BA:1022:G:C5    | 35:BA:1141:U:C4    | 3.03                     | 0.45              |
| 35:BA:1375:C:HO2'  | 35:BA:1376:C:H5'   | 1.75                     | 0.45              |
| 35:BA:1529:G:N1    | 35:BA:1541:G:N2    | 2.64                     | 0.45              |
| 35:BA:1771:C:O4'   | 35:BA:1786:A:H8    | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2137:C:O2'   | 35:BA:2138:C:OP1   | 2.34                     | 0.45              |
| 35:BA:2205:C:O5'   | 35:BA:2205:C:H6    | 1.99                     | 0.45              |
| 35:BA:438:G:O2'    | 35:BA:440:G:H5'    | 2.16                     | 0.45              |
| 38:BD:35:LYS:CA    | 38:BD:35:LYS:HZ2   | 2.29                     | 0.45              |
| 41:BG:103:LEU:HD13 | 41:BG:103:LEU:C    | 2.36                     | 0.45              |
| 41:BG:40:ASN:ND2   | 41:BG:91:ARG:HG3   | 2.31                     | 0.45              |
| 41:BG:43:LEU:O     | 41:BG:44:GLY:O     | 2.34                     | 0.45              |
| 48:BP:81:GLN:CD    | 48:BP:106:LEU:HA   | 2.36                     | 0.45              |
| 50:BR:7:GLY:C      | 50:BR:8:ARG:NE     | 2.70                     | 0.45              |
| 53:BU:57:PHE:O     | 53:BU:58:ARG:C     | 2.54                     | 0.45              |
| 35:BA:1155:A:OP2   | 53:BU:58:ARG:NH1   | 2.50                     | 0.45              |
| 58:BZ:124:ILE:O    | 58:BZ:126:VAL:HG13 | 2.16                     | 0.45              |
| 1:AA:1151:A:O2'    | 1:AA:1152:A:P      | 2.74                     | 0.45              |
| 1:AA:951:G:C6      | 1:AA:1230:C:N3     | 2.85                     | 0.45              |
| 1:AA:1285:A:H8     | 1:AA:1285:A:O5'    | 1.98                     | 0.45              |
| 1:AA:1324:A:H2'    | 1:AA:1325:C:H6     | 1.81                     | 0.45              |
| 1:AA:1347:G:N2     | 1:AA:1373:G:H2'    | 2.30                     | 0.45              |
| 1:AA:1402:C:OP2    | 23:AX:19:A:O3'     | 2.19                     | 0.45              |
| 1:AA:1407:C:H2'    | 1:AA:1408:A:C5'    | 2.46                     | 0.45              |
| 1:AA:495:A:HO2'    | 1:AA:496:A:P       | 2.40                     | 0.45              |
| 1:AA:684:A:H2'     | 1:AA:685:G:C8      | 2.50                     | 0.45              |
| 1:AA:73:G:H5'      | 1:AA:76:C:OP2      | 2.16                     | 0.45              |
| 1:AA:797:C:H2'     | 1:AA:798:G:H8      | 1.81                     | 0.45              |
| 1:AA:937:A:H2'     | 1:AA:938:A:C5'     | 2.46                     | 0.45              |
| 1:AA:959:A:C3'     | 1:AA:960:U:H4'     | 2.46                     | 0.45              |
| 2:AB:16:HIS:CE1    | 2:AB:210:SER:C     | 2.89                     | 0.45              |
| 3:AC:117:ALA:O     | 3:AC:187:ALA:HB2   | 2.16                     | 0.45              |
| 3:AC:165:THR:HG22  | 3:AC:165:THR:O     | 2.15                     | 0.45              |
| 3:AC:5:ILE:HD13    | 3:AC:5:ILE:H       | 1.82                     | 0.45              |
| 3:AC:86:VAL:HG23   | 3:AC:87:LEU:N      | 2.30                     | 0.45              |
| 4:AD:122:ARG:NH1   | 4:AD:134:ASP:OD2   | 2.49                     | 0.45              |
| 4:AD:162:LEU:HG    | 4:AD:181:MET:HE2   | 1.99                     | 0.45              |
| 6:AF:40:VAL:HG13   | 6:AF:40:VAL:O      | 2.16                     | 0.45              |
| 13:AM:82:MET:SD    | 13:AM:93:ARG:HG3   | 2.57                     | 0.45              |
| 18:AR:29:PHE:CD2   | 18:AR:39:VAL:HG11  | 2.50                     | 0.45              |
| 24:AY:138:LYS:HG2  | 61:AY:701:GCP:N1   | 2.31                     | 0.45              |
| 24:AY:510:VAL:CG1  | 24:AY:567:LEU:HD11 | 2.46                     | 0.45              |
| 24:AY:74:TRP:NE1   | 24:AY:273:LEU:HB3  | 2.31                     | 0.45              |
| 28:B3:2:PRO:O      | 28:B3:39:ASP:HB2   | 2.15                     | 0.45              |
| 31:B6:17:LYS:CA    | 31:B6:17:LYS:HE2   | 2.39                     | 0.45              |
| 32:B7:43:THR:O     | 32:B7:44:PRO:C     | 2.53                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:B8:4:MET:CG     | 33:B8:61:LEU:HD23  | 2.44                     | 0.45              |
| 35:BA:99:U:H4'     | 35:BA:102:G:H1'    | 1.98                     | 0.45              |
| 35:BA:1412:A:C2'   | 35:BA:1413:G:C5'   | 2.89                     | 0.45              |
| 35:BA:2115:G:C5'   | 35:BA:2116:G:OP2   | 2.64                     | 0.45              |
| 35:BA:2606:C:N3    | 35:BA:2607:G:N7    | 2.64                     | 0.45              |
| 35:BA:654(P):C:O2' | 35:BA:654(Q):C:H5' | 2.15                     | 0.45              |
| 37:BC:37:LYS:O     | 37:BC:38:PHE:HB3   | 2.17                     | 0.45              |
| 39:BE:119:ARG:HG3  | 39:BE:160:TYR:HB2  | 1.99                     | 0.45              |
| 39:BE:34:VAL:HG11  | 39:BE:78:LEU:HD23  | 1.98                     | 0.45              |
| 39:BE:34:VAL:HG22  | 39:BE:48:GLN:NE2   | 2.30                     | 0.45              |
| 40:BF:155:LEU:HD22 | 40:BF:186:ILE:HA   | 1.98                     | 0.45              |
| 36:BB:42:C:H5''    | 41:BG:67:LYS:HE3   | 1.97                     | 0.45              |
| 42:BH:154:PRO:C    | 42:BH:156:ALA:H    | 2.19                     | 0.45              |
| 35:BA:2531:A:H4'   | 42:BH:157:TYR:CD2  | 2.51                     | 0.45              |
| 42:BH:166:GLY:O    | 42:BH:167:GLU:HG3  | 2.16                     | 0.45              |
| 42:BH:19:VAL:O     | 42:BH:23:ARG:O     | 2.34                     | 0.45              |
| 43:BJ:98:UNK:C     | 43:BJ:100:UNK:N    | 2.77                     | 0.45              |
| 45:BL:70:UNK:O     | 45:BL:71:UNK:C     | 2.65                     | 0.45              |
| 51:BS:106:ARG:C    | 51:BS:108:GLY:H    | 2.20                     | 0.45              |
| 51:BS:35:ILE:CD1   | 51:BS:99:LYS:HD3   | 2.45                     | 0.45              |
| 57:BY:44:ILE:CG2   | 57:BY:45:VAL:H     | 2.28                     | 0.45              |
| 58:BZ:31:ARG:HD2   | 58:BZ:94:GLU:OE1   | 2.17                     | 0.45              |
| 1:AA:1178:G:H8     | 1:AA:1178:G:O5'    | 1.99                     | 0.45              |
| 1:AA:1178:G:C4     | 1:AA:1180:A:OP2    | 2.69                     | 0.45              |
| 1:AA:1202:G:H1'    | 14:AN:29:ARG:HD3   | 1.98                     | 0.45              |
| 1:AA:1258:G:O2'    | 1:AA:1259:C:H5'    | 2.15                     | 0.45              |
| 1:AA:1307:U:O2'    | 1:AA:1308:U:H5'    | 2.16                     | 0.45              |
| 1:AA:1324:A:C4'    | 1:AA:1362:C:H4'    | 2.46                     | 0.45              |
| 1:AA:343:U:H6      | 1:AA:343:U:O5'     | 1.99                     | 0.45              |
| 1:AA:356:A:C2'     | 1:AA:368:U:O2'     | 2.64                     | 0.45              |
| 1:AA:444:C:H2'     | 1:AA:445:G:H8      | 1.80                     | 0.45              |
| 1:AA:938:A:O2'     | 1:AA:939:G:C5'     | 2.55                     | 0.45              |
| 2:AB:178:ARG:NH1   | 8:AH:71:GLY:O      | 2.49                     | 0.45              |
| 2:AB:76:GLN:O      | 2:AB:211:ILE:CD1   | 2.65                     | 0.45              |
| 4:AD:170:VAL:CG1   | 4:AD:174:LEU:HB2   | 2.46                     | 0.45              |
| 7:AG:113:GLU:OE1   | 7:AG:113:GLU:N     | 2.43                     | 0.45              |
| 7:AG:5:ARG:HE      | 7:AG:5:ARG:HB2     | 1.43                     | 0.45              |
| 8:AH:112:LEU:CD2   | 8:AH:133:LEU:HD13  | 2.46                     | 0.45              |
| 9:AI:23:ASN:ND2    | 9:AI:23:ASN:N      | 2.38                     | 0.45              |
| 10:AJ:89:ASP:HB3   | 10:AJ:91:PRO:HD3   | 1.99                     | 0.45              |
| 12:AL:27:LEU:CB    | 12:AL:62:SER:HB2   | 2.46                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:AF:97:PHE:CD2   | 18:AR:31:LEU:HD21  | 2.46                     | 0.45              |
| 19:AS:53:ASN:N    | 19:AS:56:GLN:O     | 2.48                     | 0.45              |
| 25:B0:20:ARG:CG   | 25:B0:20:ARG:HH11  | 2.29                     | 0.45              |
| 26:B1:11:ARG:CB   | 26:B1:12:PRO:HD2   | 2.40                     | 0.45              |
| 26:B1:49:VAL:HG12 | 26:B1:62:VAL:HG12  | 1.98                     | 0.45              |
| 29:B4:21:VAL:O    | 29:B4:22:ILE:O     | 2.34                     | 0.45              |
| 29:B4:48:ARG:HH11 | 29:B4:48:ARG:CG    | 2.29                     | 0.45              |
| 32:B7:11:LYS:CE   | 35:BA:686:G:H5''   | 2.46                     | 0.45              |
| 35:BA:1058:G:N2   | 35:BA:1059:G:H1'   | 2.32                     | 0.45              |
| 35:BA:1936:A:OP1  | 35:BA:1937:A:H5'   | 2.16                     | 0.45              |
| 35:BA:2287:A:C2   | 35:BA:2346:A:N1    | 2.85                     | 0.45              |
| 35:BA:247:G:H3'   | 35:BA:249:C:H5     | 1.78                     | 0.45              |
| 35:BA:2680:C:O2'  | 35:BA:2681:C:H5'   | 2.17                     | 0.45              |
| 35:BA:651:G:H2'   | 35:BA:652:C:C5'    | 2.46                     | 0.45              |
| 35:BA:659:C:H2'   | 35:BA:660:G:H8     | 1.82                     | 0.45              |
| 35:BA:997:G:O2'   | 35:BA:998:C:H5'    | 2.16                     | 0.45              |
| 37:BC:23:ILE:HG12 | 37:BC:229:SER:OXT  | 2.16                     | 0.45              |
| 38:BD:34:VAL:O    | 38:BD:64:ILE:HG23  | 2.16                     | 0.45              |
| 38:BD:65:ILE:HD11 | 38:BD:67:PHE:CZ    | 2.51                     | 0.45              |
| 40:BF:82:ILE:O    | 40:BF:83:PHE:O     | 2.33                     | 0.45              |
| 42:BH:154:PRO:CB  | 42:BH:163:TYR:CZ   | 2.99                     | 0.45              |
| 48:BP:48:PRO:O    | 48:BP:50:ARG:N     | 2.50                     | 0.45              |
| 50:BR:45:ARG:CG   | 50:BR:46:GLY:N     | 2.72                     | 0.45              |
| 51:BS:89:ARG:CG   | 51:BS:92:TYR:CA    | 2.94                     | 0.45              |
| 54:BV:19:LYS:HE2  | 54:BV:19:LYS:HA    | 1.98                     | 0.45              |
| 54:BV:38:LEU:C    | 54:BV:38:LEU:HD23  | 2.36                     | 0.45              |
| 1:AA:113:G:H2'    | 1:AA:114:U:H6      | 1.78                     | 0.45              |
| 1:AA:1314:C:OP2   | 19:AS:6:LYS:CD     | 2.65                     | 0.45              |
| 1:AA:1499:A:H1'   | 1:AA:1520:G:H5'    | 1.96                     | 0.45              |
| 1:AA:159:G:H22    | 1:AA:163:C:H42     | 1.64                     | 0.45              |
| 1:AA:189(I):G:O2' | 1:AA:189(J):G:H5'  | 2.16                     | 0.45              |
| 1:AA:368:U:P      | 24:AY:351:ARG:HH21 | 2.39                     | 0.45              |
| 1:AA:495:A:O4'    | 1:AA:496:A:H8      | 1.93                     | 0.45              |
| 1:AA:507:C:H3'    | 1:AA:507:C:H6      | 1.82                     | 0.45              |
| 2:AB:114:ARG:CG   | 2:AB:114:ARG:NH1   | 2.77                     | 0.45              |
| 4:AD:157:LEU:HG   | 4:AD:161:ASN:ND2   | 2.32                     | 0.45              |
| 10:AJ:32:ALA:CB   | 10:AJ:81:THR:HG21  | 2.47                     | 0.45              |
| 12:AL:109:GLY:HA3 | 12:AL:121:GLY:O    | 2.17                     | 0.45              |
| 12:AL:48:PRO:HG2  | 12:AL:49:ASN:H     | 1.81                     | 0.45              |
| 13:AM:10:PRO:O    | 13:AM:11:ARG:CB    | 2.63                     | 0.45              |
| 22:AV:47:U:H3'    | 22:AV:48:C:C5'     | 2.46                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:AY:137:ASN:CG   | 24:AY:138:LYS:H   | 2.18                     | 0.45              |
| 24:AY:500:GLN:O    | 24:AY:500:GLN:NE2 | 2.38                     | 0.45              |
| 24:AY:491:VAL:HG21 | 24:AY:597:GLY:HA2 | 1.97                     | 0.45              |
| 28:B3:35:ARG:HD3   | 28:B3:37:LEU:CD2  | 2.41                     | 0.45              |
| 35:BA:70:G:H5''    | 35:BA:112:U:O2    | 2.17                     | 0.45              |
| 35:BA:1290:C:HO2'  | 35:BA:1291:C:H5'  | 1.80                     | 0.45              |
| 35:BA:1291:C:O2'   | 35:BA:1292:U:C5'  | 2.52                     | 0.45              |
| 35:BA:1646:C:H6    | 35:BA:1646:C:O5'  | 2.00                     | 0.45              |
| 35:BA:1786:A:C4    | 35:BA:1938:A:N6   | 2.84                     | 0.45              |
| 35:BA:1981:A:H5''  | 35:BA:1982:C:OP2  | 2.16                     | 0.45              |
| 35:BA:2009:G:C2    | 35:BA:2010:G:N7   | 2.84                     | 0.45              |
| 35:BA:2887:U:H2'   | 35:BA:2888:C:H6   | 1.81                     | 0.45              |
| 35:BA:43:A:O5'     | 35:BA:43:A:H8     | 2.00                     | 0.45              |
| 35:BA:491:G:H2'    | 35:BA:492:A:H8    | 1.81                     | 0.45              |
| 35:BA:885:C:O2     | 35:BA:886:C:N4    | 2.50                     | 0.45              |
| 36:BB:13:A:H5'     | 36:BB:13:A:H8     | 1.82                     | 0.45              |
| 36:BB:34:U:H5      | 41:BG:96:ARG:HH12 | 1.63                     | 0.45              |
| 37:BC:48:LEU:HD23  | 37:BC:59:VAL:HG21 | 1.98                     | 0.45              |
| 38:BD:206:LEU:HD23 | 38:BD:206:LEU:HA  | 1.78                     | 0.45              |
| 38:BD:211:ARG:O    | 38:BD:215:LEU:HG  | 2.17                     | 0.45              |
| 39:BE:120:TRP:O    | 39:BE:122:PHE:N   | 2.50                     | 0.45              |
| 44:BK:30:UNK:O     | 44:BK:31:UNK:C    | 2.64                     | 0.45              |
| 49:BQ:135:ASP:H    | 49:BQ:137:TYR:HD2 | 1.59                     | 0.45              |
| 51:BS:12:PHE:HD1   | 51:BS:12:PHE:C    | 2.20                     | 0.45              |
| 52:BT:34:VAL:HG11  | 52:BT:39:ARG:HG3  | 1.97                     | 0.45              |
| 52:BT:91:ARG:O     | 52:BT:92:GLY:C    | 2.54                     | 0.45              |
| 52:BT:95:ARG:CB    | 52:BT:95:ARG:HH11 | 2.30                     | 0.45              |
| 52:BT:95:ARG:HB3   | 52:BT:95:ARG:CZ   | 2.47                     | 0.45              |
| 53:BU:68:ALA:O     | 53:BU:71:GLN:HG3  | 2.17                     | 0.45              |
| 54:BV:52:VAL:HG13  | 54:BV:55:ALA:HB3  | 1.98                     | 0.45              |
| 56:BX:57:LEU:HD22  | 56:BX:57:LEU:O    | 2.15                     | 0.45              |
| 57:BY:60:PHE:O     | 57:BY:61:ILE:HG13 | 2.15                     | 0.45              |
| 58:BZ:48:PHE:CD1   | 58:BZ:52:SER:HA   | 2.51                     | 0.45              |
| 1:AA:1447:A:OP2    | 1:AA:1447:A:H4'   | 2.16                     | 0.45              |
| 1:AA:744:C:H2'     | 1:AA:745:C:C6     | 2.52                     | 0.45              |
| 1:AA:941:G:O2'     | 1:AA:942:G:O5'    | 2.34                     | 0.45              |
| 2:AB:11:LEU:HD13   | 2:AB:217:ARG:NH2  | 2.32                     | 0.45              |
| 3:AC:65:ALA:O      | 3:AC:66:VAL:HB    | 2.17                     | 0.45              |
| 4:AD:107:ARG:HH11  | 4:AD:107:ARG:HG2  | 1.82                     | 0.45              |
| 6:AF:41:GLU:HG3    | 6:AF:62:TRP:CE3   | 2.52                     | 0.45              |
| 16:AP:57:ARG:HG3   | 16:AP:79:VAL:HG13 | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:600:VAL:HG21 | 24:AY:678:GLU:OE1  | 2.16                     | 0.45              |
| 33:B8:48:PHE:C     | 33:B8:49:VAL:CG2   | 2.84                     | 0.45              |
| 35:BA:1243:G:H2'   | 35:BA:1244:G:O4'   | 2.16                     | 0.45              |
| 35:BA:1336:A:O2'   | 35:BA:1337:G:H5'   | 2.16                     | 0.45              |
| 35:BA:1422:G:C4    | 35:BA:1423:G:N7    | 2.85                     | 0.45              |
| 35:BA:1688:U:H5'   | 35:BA:1689:A:OP1   | 2.15                     | 0.45              |
| 35:BA:2007:C:C2'   | 35:BA:2008:C:H5'   | 2.40                     | 0.45              |
| 35:BA:2009:G:C3'   | 35:BA:2010:G:C5'   | 2.95                     | 0.45              |
| 35:BA:2688:U:H5    | 35:BA:2720:U:OP2   | 2.00                     | 0.45              |
| 35:BA:477:A:H2'    | 35:BA:478:A:C8     | 2.52                     | 0.45              |
| 35:BA:654(N):G:H2' | 35:BA:654(O):G:C4' | 2.46                     | 0.45              |
| 35:BA:79:G:O2'     | 35:BA:80:G:H5'     | 2.17                     | 0.45              |
| 37:BC:104:ILE:O    | 37:BC:105:LEU:C    | 2.55                     | 0.45              |
| 37:BC:139:PRO:HB2  | 37:BC:146:VAL:HG22 | 1.97                     | 0.45              |
| 40:BF:185:ASP:OD1  | 40:BF:188:ARG:HD3  | 2.17                     | 0.45              |
| 41:BG:130:ASN:O    | 41:BG:159:VAL:O    | 2.34                     | 0.45              |
| 48:BP:51:PHE:CG    | 48:BP:52:GLU:O     | 2.69                     | 0.45              |
| 35:BA:956:G:P      | 49:BQ:14:ARG:HH21  | 2.38                     | 0.45              |
| 51:BS:83:LYS:HG2   | 51:BS:105:ALA:CB   | 2.47                     | 0.45              |
| 51:BS:89:ARG:NH1   | 51:BS:92:TYR:HA    | 2.31                     | 0.45              |
| 54:BV:39:LEU:HD22  | 54:BV:39:LEU:N     | 2.31                     | 0.45              |
| 55:BW:26:GLY:H     | 55:BW:71:VAL:CG2   | 2.22                     | 0.45              |
| 1:AA:1279:A:H2'    | 1:AA:1282:C:H42    | 1.80                     | 0.45              |
| 1:AA:1285:A:O2'    | 1:AA:1286:A:OP2    | 2.35                     | 0.45              |
| 1:AA:1288:A:H1'    | 1:AA:1352:C:O2'    | 2.17                     | 0.45              |
| 1:AA:1310:G:O2'    | 1:AA:1311:G:H5'    | 2.16                     | 0.45              |
| 1:AA:1442:G:H22    | 1:AA:1461:G:H21    | 1.65                     | 0.45              |
| 1:AA:161:A:H2'     | 1:AA:162:A:H8      | 1.81                     | 0.45              |
| 1:AA:773:G:C2      | 1:AA:774:G:C4      | 3.05                     | 0.45              |
| 1:AA:863:U:O2      | 1:AA:863:U:C3'     | 2.65                     | 0.45              |
| 1:AA:943:U:H6      | 1:AA:943:U:O5'     | 1.98                     | 0.45              |
| 2:AB:61:LEU:HD11   | 2:AB:160:ASP:HB2   | 1.97                     | 0.45              |
| 3:AC:95:THR:C      | 3:AC:97:LYS:H      | 2.18                     | 0.45              |
| 7:AG:70:LYS:CB     | 7:AG:100:ALA:HB2   | 2.46                     | 0.45              |
| 7:AG:7:ALA:O       | 7:AG:8:GLU:HB3     | 2.17                     | 0.45              |
| 9:AI:78:LYS:HE2    | 9:AI:101:PHE:HA    | 1.99                     | 0.45              |
| 13:AM:22:ILE:HB    | 13:AM:25:ILE:HB    | 1.98                     | 0.45              |
| 13:AM:81:LEU:O     | 13:AM:89:GLY:HA3   | 2.16                     | 0.45              |
| 1:AA:275:G:H5'     | 17:AQ:14:LYS:CD    | 2.47                     | 0.45              |
| 17:AQ:86:GLU:O     | 17:AQ:90:ILE:HG12  | 2.17                     | 0.45              |
| 19:AS:31:ILE:HG23  | 19:AS:31:ILE:O     | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:181:LEU:HD23 | 24:AY:182:ARG:CZ   | 2.47                     | 0.45              |
| 25:B0:50:ASN:CG    | 25:B0:63:VAL:HG21  | 2.37                     | 0.45              |
| 28:B3:35:ARG:HG2   | 28:B3:36:VAL:N     | 2.31                     | 0.45              |
| 29:B4:24:THR:O     | 29:B4:25:TYR:CB    | 2.65                     | 0.45              |
| 29:B4:2:LYS:CE     | 29:B4:4:GLY:O      | 2.60                     | 0.45              |
| 30:B5:8:LYS:O      | 35:BA:2017:U:H4'   | 2.16                     | 0.45              |
| 33:B8:45:GLY:O     | 33:B8:46:ARG:HB2   | 2.17                     | 0.45              |
| 34:B9:10:ILE:O     | 34:B9:11:CYS:CB    | 2.61                     | 0.45              |
| 35:BA:111:A:O2'    | 35:BA:112:U:H5''   | 2.15                     | 0.45              |
| 35:BA:1298:C:O2'   | 35:BA:1301:A:H1'   | 2.16                     | 0.45              |
| 35:BA:1336:A:H2'   | 35:BA:1337:G:H8    | 1.82                     | 0.45              |
| 35:BA:1407:C:H5'   | 35:BA:1408:C:OP2   | 2.14                     | 0.45              |
| 35:BA:1504:C:HO2'  | 35:BA:1505:C:P     | 2.40                     | 0.45              |
| 35:BA:1670:C:O2    | 39:BE:129:HIS:HE1  | 1.99                     | 0.45              |
| 35:BA:1770:G:O2'   | 35:BA:1771:C:C5'   | 2.43                     | 0.45              |
| 35:BA:49:A:C6      | 35:BA:177:G:C2     | 3.04                     | 0.45              |
| 35:BA:1820:U:N3    | 38:BD:160:GLY:HA3  | 2.31                     | 0.45              |
| 35:BA:1967:C:C4    | 35:BA:1968:G:C5    | 3.04                     | 0.45              |
| 35:BA:2012:G:O3'   | 55:BW:96:ILE:HG13  | 2.16                     | 0.45              |
| 35:BA:2389:G:H5''  | 35:BA:2390:U:O4'   | 2.17                     | 0.45              |
| 35:BA:2555:U:C3'   | 35:BA:2556:C:C5'   | 2.90                     | 0.45              |
| 35:BA:271(M):G:H3' | 35:BA:271(M):G:H8  | 1.80                     | 0.45              |
| 35:BA:2864:G:H2'   | 35:BA:2865:U:C6    | 2.51                     | 0.45              |
| 35:BA:607:U:O2     | 35:BA:621:A:N1     | 2.50                     | 0.45              |
| 35:BA:884:C:N4     | 35:BA:892:G:N1     | 2.61                     | 0.45              |
| 37:BC:203:GLU:N    | 37:BC:203:GLU:CD   | 2.70                     | 0.45              |
| 38:BD:108:PRO:HG2  | 38:BD:111:LEU:CB   | 2.40                     | 0.45              |
| 41:BG:106:LEU:C    | 41:BG:106:LEU:HD23 | 2.37                     | 0.45              |
| 41:BG:110:ALA:HB1  | 41:BG:142:PRO:HG3  | 1.98                     | 0.45              |
| 41:BG:113:ARG:NE   | 41:BG:113:ARG:CA   | 2.80                     | 0.45              |
| 41:BG:180:PHE:CD1  | 41:BG:181:ARG:HG2  | 2.51                     | 0.45              |
| 41:BG:77:ILE:HG21  | 41:BG:81:LYS:N     | 2.31                     | 0.45              |
| 44:BK:109:UNK:C    | 44:BK:111:UNK:N    | 2.80                     | 0.45              |
| 48:BP:82:GLY:HA2   | 48:BP:113:LYS:O    | 2.16                     | 0.45              |
| 51:BS:20:ARG:NE    | 51:BS:20:ARG:CA    | 2.80                     | 0.45              |
| 1:AA:346:G:H5'     | 52:BT:35:LYS:HZ1   | 1.80                     | 0.45              |
| 52:BT:40:THR:O     | 52:BT:41:ARG:HB3   | 2.17                     | 0.45              |
| 53:BU:114:LYS:HG2  | 53:BU:114:LYS:H    | 1.57                     | 0.45              |
| 53:BU:95:LEU:HD13  | 54:BV:4:ILE:CG2    | 2.46                     | 0.45              |
| 54:BV:52:VAL:HG13  | 54:BV:52:VAL:O     | 2.16                     | 0.45              |
| 57:BY:13:VAL:HG22  | 57:BY:14:LEU:H     | 1.80                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:BY:17:SER:CB   | 57:BY:71:LYS:HB3   | 2.46                     | 0.45              |
| 58:BZ:104:PHE:HB3 | 58:BZ:141:VAL:CG2  | 2.43                     | 0.45              |
| 58:BZ:62:PRO:C    | 58:BZ:64:GLY:H     | 2.20                     | 0.45              |
| 1:AA:1077:G:C6    | 1:AA:1081:G:C6     | 3.03                     | 0.45              |
| 1:AA:1457:G:OP1   | 20:AT:39:LYS:NZ    | 2.50                     | 0.45              |
| 1:AA:1498:U:C1'   | 1:AA:1499:A:P      | 3.05                     | 0.45              |
| 1:AA:189(B):C:O2' | 1:AA:189(C):C:H5'  | 2.16                     | 0.45              |
| 1:AA:81:U:H2'     | 1:AA:88:A:H61      | 1.81                     | 0.45              |
| 2:AB:113:HIS:HA   | 2:AB:116:GLU:HG3   | 1.98                     | 0.45              |
| 2:AB:124:SER:HB2  | 2:AB:125:PRO:CD    | 2.46                     | 0.45              |
| 2:AB:15:VAL:CG1   | 2:AB:209:ARG:HB3   | 2.46                     | 0.45              |
| 2:AB:21:ARG:HB3   | 2:AB:38:GLY:O      | 2.17                     | 0.45              |
| 2:AB:67:THR:HA    | 2:AB:90:MET:SD     | 2.57                     | 0.45              |
| 4:AD:61:LYS:NZ    | 4:AD:62:GLN:NE2    | 2.65                     | 0.45              |
| 4:AD:63:LYS:HD3   | 4:AD:197:PRO:O     | 2.17                     | 0.45              |
| 8:AH:105:ARG:HD3  | 8:AH:105:ARG:HA    | 1.63                     | 0.45              |
| 1:AA:1314:C:H5    | 19:AS:6:LYS:CE     | 2.30                     | 0.45              |
| 20:AT:75:ASN:HA   | 20:AT:78:ALA:HB3   | 1.99                     | 0.45              |
| 24:AY:190:ASN:C   | 24:AY:192:LEU:H    | 2.20                     | 0.45              |
| 24:AY:232:LEU:H   | 24:AY:232:LEU:HD13 | 1.81                     | 0.45              |
| 25:B0:23:VAL:HG22 | 25:B0:38:VAL:HG22  | 1.98                     | 0.45              |
| 27:B2:33:MET:HG3  | 27:B2:36:ARG:NH2   | 2.31                     | 0.45              |
| 35:BA:1105:U:O2'  | 35:BA:1106:G:OP2   | 2.30                     | 0.45              |
| 35:BA:1132:A:C2'  | 35:BA:1133:U:H5'   | 2.46                     | 0.45              |
| 35:BA:1140:C:H2'  | 35:BA:1141:U:H5'   | 1.98                     | 0.45              |
| 35:BA:1422:G:C4   | 35:BA:1423:G:C8    | 3.04                     | 0.45              |
| 35:BA:1517:G:H2'  | 35:BA:1518:U:O4'   | 2.16                     | 0.45              |
| 35:BA:1786:A:C1'  | 35:BA:1938:A:H61   | 2.26                     | 0.45              |
| 30:B5:2:ALA:HA    | 35:BA:2015:A:O4'   | 2.17                     | 0.45              |
| 35:BA:2030:A:H4'  | 35:BA:2031:A:C8    | 2.52                     | 0.45              |
| 35:BA:2078:C:H2'  | 35:BA:2079:U:C6    | 2.51                     | 0.45              |
| 35:BA:2134:A:C8   | 35:BA:2134:A:H5'   | 2.49                     | 0.45              |
| 35:BA:2305:A:H2   | 35:BA:2306:C:H1'   | 1.80                     | 0.45              |
| 35:BA:2410:G:H2'  | 35:BA:2411:A:O4'   | 2.17                     | 0.45              |
| 35:BA:2602:A:OP2  | 35:BA:2602:A:H4'   | 2.16                     | 0.45              |
| 35:BA:2612:C:H2'  | 35:BA:2613:U:H5'   | 1.98                     | 0.45              |
| 35:BA:610:G:H2'   | 35:BA:611:C:C6     | 2.52                     | 0.45              |
| 35:BA:743:G:C2'   | 35:BA:744:G:C8     | 2.68                     | 0.45              |
| 35:BA:773:U:C5'   | 38:BD:47:GLY:HA3   | 2.46                     | 0.45              |
| 35:BA:995:C:C2    | 53:BU:57:PHE:HE2   | 2.35                     | 0.45              |
| 37:BC:138:LEU:O   | 37:BC:139:PRO:C    | 2.53                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BC:211:ARG:HG2  | 37:BC:211:ARG:HH11 | 1.81                     | 0.45              |
| 37:BC:22:THR:HG23  | 37:BC:25:GLU:OE1   | 2.17                     | 0.45              |
| 38:BD:142:VAL:HG21 | 38:BD:191:ALA:CB   | 2.47                     | 0.45              |
| 35:BA:1658:C:OP1   | 39:BE:132:HIS:ND1  | 2.49                     | 0.45              |
| 40:BF:9:ILE:HA     | 40:BF:14:PRO:HA    | 1.98                     | 0.45              |
| 40:BF:160:ASN:HD21 | 40:BF:162:LEU:CD1  | 2.18                     | 0.45              |
| 29:B4:32:TYR:CD2   | 41:BG:113:ARG:HD2  | 2.51                     | 0.45              |
| 41:BG:19:LEU:O     | 41:BG:21:ARG:N     | 2.50                     | 0.45              |
| 42:BH:44:VAL:HG12  | 42:BH:45:VAL:N     | 2.32                     | 0.45              |
| 44:BK:117:UNK:O    | 44:BK:119:UNK:N    | 2.49                     | 0.45              |
| 49:BQ:17:LEU:CD2   | 49:BQ:96:VAL:HG13  | 2.44                     | 0.45              |
| 50:BR:103:ARG:HH12 | 50:BR:110:PRO:CD   | 2.27                     | 0.45              |
| 50:BR:33:ARG:HG3   | 50:BR:115:GLU:HG3  | 1.97                     | 0.45              |
| 52:BT:39:ARG:N     | 52:BT:39:ARG:HD2   | 2.29                     | 0.45              |
| 53:BU:95:LEU:C     | 53:BU:97:ASP:N     | 2.69                     | 0.45              |
| 58:BZ:53:ILE:HG13  | 58:BZ:54:HIS:CD2   | 2.52                     | 0.45              |
| 1:AA:1029:C:C2'    | 1:AA:1030:C:H5''   | 2.46                     | 0.45              |
| 1:AA:1119:C:O2'    | 1:AA:1120:G:H5'    | 2.17                     | 0.45              |
| 1:AA:159:G:H22     | 1:AA:163:C:N4      | 2.14                     | 0.45              |
| 1:AA:180:U:C2'     | 1:AA:181:G:H5'     | 2.47                     | 0.45              |
| 1:AA:335:C:H2'     | 1:AA:336:C:C6      | 2.52                     | 0.45              |
| 2:AB:107:THR:O     | 2:AB:110:GLN:HG2   | 2.17                     | 0.45              |
| 3:AC:129:ALA:HB1   | 3:AC:133:ALA:H     | 1.82                     | 0.45              |
| 3:AC:43:LEU:O      | 3:AC:47:LEU:HB2    | 2.17                     | 0.45              |
| 7:AG:113:GLU:HB3   | 7:AG:118:VAL:CG1   | 2.47                     | 0.45              |
| 9:AI:10:ARG:CD     | 9:AI:105:ASP:HB3   | 2.47                     | 0.45              |
| 14:AN:33:VAL:O     | 14:AN:33:VAL:CG2   | 2.64                     | 0.45              |
| 20:AT:26:ASN:CB    | 20:AT:71:THR:OG1   | 2.62                     | 0.45              |
| 1:AA:188:C:O4'     | 20:AT:89:ARG:NH1   | 2.49                     | 0.45              |
| 24:AY:105:ILE:N    | 24:AY:105:ILE:HD12 | 2.31                     | 0.45              |
| 24:AY:517:LEU:HD11 | 24:AY:564:LYS:N    | 2.31                     | 0.45              |
| 24:AY:96:ARG:O     | 24:AY:100:VAL:HG12 | 2.17                     | 0.45              |
| 25:B0:15:ASP:OD1   | 25:B0:16:SER:N     | 2.41                     | 0.45              |
| 25:B0:26:TYR:CD1   | 25:B0:26:TYR:N     | 2.84                     | 0.45              |
| 25:B0:67:VAL:O     | 25:B0:68:GLU:HB3   | 2.16                     | 0.45              |
| 26:B1:52:ARG:C     | 26:B1:53:VAL:HG13  | 2.36                     | 0.45              |
| 26:B1:64:ALA:HA    | 26:B1:67:ILE:CD1   | 2.47                     | 0.45              |
| 27:B2:51:ARG:HE    | 27:B2:51:ARG:HB2   | 1.52                     | 0.45              |
| 29:B4:27:THR:OG1   | 29:B4:27:THR:O     | 2.31                     | 0.45              |
| 30:B5:2:ALA:N      | 35:BA:747:U:C5     | 2.85                     | 0.45              |
| 35:BA:1041:G:H1    | 35:BA:1114:G:N2    | 2.15                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:1120:G:H2'  | 35:BA:1121:C:H6    | 1.82                     | 0.45              |
| 35:BA:1138:G:O2'  | 46:BN:102:ALA:O    | 2.34                     | 0.45              |
| 35:BA:1922:G:O2'  | 35:BA:1923:U:H5'   | 2.16                     | 0.45              |
| 35:BA:1992:G:H5'  | 35:BA:1994:C:N4    | 2.32                     | 0.45              |
| 35:BA:201:C:O2'   | 35:BA:202:U:H5'    | 2.17                     | 0.45              |
| 35:BA:2695:C:H2'  | 35:BA:2696:U:H6    | 1.82                     | 0.45              |
| 35:BA:318:C:H2'   | 35:BA:319:C:H6     | 1.82                     | 0.45              |
| 35:BA:324:A:H2'   | 35:BA:325:G:O4'    | 2.17                     | 0.45              |
| 35:BA:673:C:H4'   | 40:BF:82:ILE:CG1   | 2.47                     | 0.45              |
| 35:BA:698:C:O2'   | 35:BA:734:A:N6     | 2.48                     | 0.45              |
| 36:BB:16:G:O2'    | 36:BB:17:C:O5'     | 2.34                     | 0.45              |
| 44:BK:8:UNK:O     | 44:BK:9:UNK:CB     | 2.64                     | 0.45              |
| 48:BP:113:LYS:HG2 | 48:BP:115:LEU:HD13 | 1.99                     | 0.45              |
| 48:BP:77:ARG:CD   | 48:BP:78:PRO:HD2   | 2.37                     | 0.45              |
| 49:BQ:42:ILE:HG12 | 49:BQ:103:MET:CE   | 2.47                     | 0.45              |
| 49:BQ:133:ARG:HG3 | 49:BQ:133:ARG:NH1  | 2.32                     | 0.45              |
| 51:BS:99:LYS:HZ3  | 51:BS:99:LYS:HB3   | 1.81                     | 0.45              |
| 53:BU:32:PHE:CB   | 53:BU:36:ARG:NH2   | 2.80                     | 0.45              |
| 35:BA:996:A:C4'   | 53:BU:92:ARG:NE    | 2.76                     | 0.45              |
| 54:BV:8:GLY:O     | 54:BV:10:LYS:HE3   | 2.17                     | 0.45              |
| 57:BY:28:LYS:CE   | 57:BY:28:LYS:N     | 2.79                     | 0.45              |
| 57:BY:81:LYS:HG3  | 57:BY:82:PRO:HD2   | 1.98                     | 0.45              |
| 58:BZ:166:SER:N   | 58:BZ:167:PRO:HA   | 2.32                     | 0.45              |
| 1:AA:1387:G:HO2'  | 1:AA:1388:C:H5'    | 1.77                     | 0.45              |
| 1:AA:1476:G:H2'   | 1:AA:1477:C:H6     | 1.81                     | 0.45              |
| 1:AA:1486:G:H2'   | 1:AA:1487:G:O4'    | 2.17                     | 0.45              |
| 1:AA:564:C:N4     | 1:AA:565:U:O4      | 2.50                     | 0.45              |
| 1:AA:591:U:H2'    | 1:AA:592:G:O5'     | 2.17                     | 0.45              |
| 1:AA:89:C:O2'     | 1:AA:90:U:C6       | 2.69                     | 0.45              |
| 2:AB:136:VAL:O    | 2:AB:140:HIS:HB2   | 2.17                     | 0.45              |
| 2:AB:163:PHE:HA   | 2:AB:185:ILE:O     | 2.17                     | 0.45              |
| 2:AB:229:VAL:HB   | 2:AB:230:VAL:H     | 1.46                     | 0.45              |
| 7:AG:30:ILE:HD13  | 7:AG:105:VAL:HG22  | 1.99                     | 0.45              |
| 1:AA:973:G:N3     | 10:AJ:55:LYS:HE3   | 2.31                     | 0.45              |
| 11:AK:15:ALA:O    | 11:AK:78:GLN:N     | 2.41                     | 0.45              |
| 1:AA:449:C:O2     | 16:AP:42:ARG:HD2   | 2.16                     | 0.45              |
| 6:AF:97:PHE:O     | 18:AR:31:LEU:HD23  | 2.17                     | 0.45              |
| 22:AV:27:G:O2'    | 22:AV:28:G:H5'     | 2.17                     | 0.45              |
| 24:AY:114:VAL:CG2 | 24:AY:152:THR:HG23 | 2.46                     | 0.45              |
| 24:AY:17:ILE:HD13 | 24:AY:81:ILE:HG22  | 1.99                     | 0.45              |
| 24:AY:29:THR:O    | 24:AY:33:LEU:HD13  | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:B2:12:GLU:O     | 27:B2:12:GLU:HG2   | 2.16                     | 0.45              |
| 31:B6:39:TYR:O     | 31:B6:41:PRO:HD3   | 2.16                     | 0.45              |
| 35:BA:1028:A:O2'   | 35:BA:1029:A:H5'   | 2.16                     | 0.45              |
| 35:BA:1055:G:H2'   | 35:BA:1056:G:O4'   | 2.16                     | 0.45              |
| 35:BA:13:A:H61     | 35:BA:525:U:H3'    | 1.82                     | 0.45              |
| 35:BA:1445:A:H8    | 35:BA:1460:A:C6    | 2.35                     | 0.45              |
| 35:BA:1494:A:O2'   | 35:BA:1495:A:H5''  | 2.17                     | 0.45              |
| 35:BA:1754:C:N3    | 35:BA:2716:U:O2'   | 2.43                     | 0.45              |
| 35:BA:1810:A:H2'   | 35:BA:1811:G:O4'   | 2.17                     | 0.45              |
| 35:BA:1999:C:H2'   | 35:BA:2000:G:C5'   | 2.40                     | 0.45              |
| 35:BA:2106:G:C8    | 35:BA:2106:G:H5'   | 2.51                     | 0.45              |
| 35:BA:2131:G:H5'   | 35:BA:2133:A:O4'   | 2.17                     | 0.45              |
| 35:BA:2332:U:H5'   | 35:BA:2336:A:N6    | 2.32                     | 0.45              |
| 35:BA:271(J):C:O2  | 35:BA:271(M):G:O6  | 2.35                     | 0.45              |
| 35:BA:271(M):G:C8  | 35:BA:271(M):G:H3' | 2.52                     | 0.45              |
| 35:BA:2748:A:C8    | 35:BA:2757:A:N6    | 2.85                     | 0.45              |
| 35:BA:2879:C:H4'   | 35:BA:2880:C:OP1   | 2.17                     | 0.45              |
| 35:BA:603:A:O4'    | 35:BA:604:G:O5'    | 2.35                     | 0.45              |
| 35:BA:61:G:H1      | 35:BA:94:C:N4      | 2.14                     | 0.45              |
| 35:BA:654(A):G:H2' | 35:BA:654(B):C:C5' | 2.47                     | 0.45              |
| 35:BA:654(U):A:H2' | 35:BA:654(V):A:C8  | 2.52                     | 0.45              |
| 35:BA:693:C:H2'    | 35:BA:694:U:O5'    | 2.17                     | 0.45              |
| 32:B7:10:ARG:NH1   | 35:BA:771:G:OP1    | 2.49                     | 0.45              |
| 35:BA:869:G:C2'    | 35:BA:870:A:H5'    | 2.47                     | 0.45              |
| 35:BA:885:C:H2'    | 35:BA:886:C:C5     | 2.52                     | 0.45              |
| 37:BC:174:ALA:HA   | 37:BC:175:PRO:HD3  | 1.81                     | 0.45              |
| 1:AA:680:C:O2'     | 38:BD:166:GLN:CG   | 2.64                     | 0.45              |
| 40:BF:39:TRP:O     | 40:BF:43:LYS:HG2   | 2.17                     | 0.45              |
| 41:BG:104:GLU:HB3  | 41:BG:105:LYS:NZ   | 2.31                     | 0.45              |
| 42:BH:89:ILE:C     | 42:BH:89:ILE:HD12  | 2.37                     | 0.45              |
| 50:BR:45:ARG:HA    | 50:BR:95:THR:HG21  | 1.97                     | 0.45              |
| 52:BT:107:ASP:CG   | 52:BT:108:ARG:H    | 2.20                     | 0.45              |
| 52:BT:30:VAL:CG1   | 52:BT:31:SER:CB    | 2.57                     | 0.45              |
| 54:BV:61:VAL:O     | 54:BV:61:VAL:CG2   | 2.64                     | 0.45              |
| 55:BW:66:GLU:O     | 55:BW:66:GLU:HG2   | 2.17                     | 0.45              |
| 1:AA:141:A:H1'     | 1:AA:182:U:O2      | 2.17                     | 0.45              |
| 1:AA:1526:G:C2'    | 1:AA:1527:C:C5'    | 2.95                     | 0.45              |
| 1:AA:1529:G:H4'    | 1:AA:1530:G:OP2    | 2.17                     | 0.45              |
| 1:AA:450:G:C5'     | 16:AP:41:PRO:O     | 2.65                     | 0.45              |
| 1:AA:486:U:H2'     | 1:AA:487:A:H8      | 1.81                     | 0.45              |
| 1:AA:627:G:H2'     | 1:AA:628:G:H8      | 1.82                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:773:G:C2'     | 1:AA:774:G:C5'    | 2.88                     | 0.45              |
| 1:AA:776:G:N2      | 1:AA:802:A:OP2    | 2.46                     | 0.45              |
| 2:AB:97:TRP:CH2    | 2:AB:176:GLU:CD   | 2.90                     | 0.45              |
| 2:AB:36:ARG:O      | 2:AB:37:ASN:HB3   | 2.16                     | 0.45              |
| 2:AB:80:ILE:HD11   | 2:AB:208:ILE:HG23 | 1.98                     | 0.45              |
| 2:AB:87:ARG:NH2    | 2:AB:233:SER:N    | 2.64                     | 0.45              |
| 2:AB:86:GLU:C      | 2:AB:88:ALA:H     | 2.20                     | 0.45              |
| 3:AC:15:THR:HG21   | 3:AC:181:ASN:HA   | 1.98                     | 0.45              |
| 5:AE:101:ILE:O     | 5:AE:120:THR:HB   | 2.18                     | 0.45              |
| 6:AF:98:LEU:N      | 6:AF:98:LEU:HD12  | 2.32                     | 0.45              |
| 10:AJ:4:ILE:CD1    | 10:AJ:4:ILE:N     | 2.80                     | 0.45              |
| 10:AJ:53:PRO:HA    | 14:AN:42:ILE:HD12 | 1.98                     | 0.45              |
| 20:AT:89:ARG:HH22  | 20:AT:106:ALA:HB2 | 1.82                     | 0.45              |
| 24:AY:554:PRO:HG2  | 24:AY:555:LEU:N   | 2.32                     | 0.45              |
| 24:AY:67:ALA:HB3   | 24:AY:83:ASP:O    | 2.17                     | 0.45              |
| 24:AY:81:ILE:O     | 24:AY:82:ILE:CG1  | 2.64                     | 0.45              |
| 35:BA:1047:G:N2    | 35:BA:1110:G:H2'  | 2.32                     | 0.45              |
| 35:BA:1146:C:O2'   | 35:BA:1147:C:H5'  | 2.17                     | 0.45              |
| 35:BA:1204:A:C2    | 35:BA:1241:A:N1   | 2.85                     | 0.45              |
| 35:BA:1317:A:H2'   | 35:BA:1318:C:C6   | 2.51                     | 0.45              |
| 35:BA:1806:C:H2'   | 35:BA:1807:G:C8   | 2.52                     | 0.45              |
| 35:BA:1806:C:H2'   | 35:BA:1807:G:H8   | 1.82                     | 0.45              |
| 35:BA:1827:C:O2'   | 35:BA:1828:G:H5'  | 2.16                     | 0.45              |
| 35:BA:2117:A:H4'   | 35:BA:2118:U:OP1  | 2.17                     | 0.45              |
| 35:BA:2124:G:H1    | 35:BA:2174:C:N4   | 2.06                     | 0.45              |
| 35:BA:289:A:H2'    | 35:BA:290:G:O4'   | 2.17                     | 0.45              |
| 35:BA:536:A:H2'    | 35:BA:537:C:H6    | 1.81                     | 0.45              |
| 35:BA:886:C:N4     | 35:BA:892:G:C2    | 2.85                     | 0.45              |
| 35:BA:94:C:H2'     | 35:BA:94:C:O2     | 2.17                     | 0.45              |
| 37:BC:179:ALA:O    | 37:BC:180:SER:O   | 2.35                     | 0.45              |
| 37:BC:16:ASP:OD2   | 37:BC:19:LYS:HB2  | 2.17                     | 0.45              |
| 38:BD:97:TYR:HB3   | 38:BD:99:ASP:HB2  | 1.99                     | 0.45              |
| 39:BE:9:VAL:HG11   | 39:BE:25:VAL:HG12 | 1.99                     | 0.45              |
| 40:BF:135:LYS:O    | 40:BF:138:GLU:N   | 2.50                     | 0.45              |
| 40:BF:125:LEU:HD12 | 40:BF:196:LEU:CD2 | 2.47                     | 0.45              |
| 40:BF:2:LYS:O      | 40:BF:3:GLU:HB3   | 2.17                     | 0.45              |
| 42:BH:83:TYR:HB2   | 42:BH:84:SER:H    | 1.49                     | 0.45              |
| 45:BL:68:UNK:HA    | 45:BL:71:UNK:CB   | 2.47                     | 0.45              |
| 49:BQ:16:ARG:CG    | 49:BQ:16:ARG:HH11 | 2.30                     | 0.45              |
| 51:BS:52:SER:O     | 51:BS:69:VAL:HG23 | 2.16                     | 0.45              |
| 52:BT:113:LYS:HA   | 52:BT:113:LYS:HD3 | 1.77                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:BU:111:GLU:HA   | 53:BU:111:GLU:OE1   | 2.16                     | 0.45              |
| 53:BU:57:PHE:HB3   | 53:BU:61:TRP:CZ2    | 2.52                     | 0.45              |
| 1:AA:1001:A:H2'    | 1:AA:1001(A):G:H5'  | 1.99                     | 0.44              |
| 1:AA:1033:G:H2'    | 1:AA:1034:G:C8      | 2.50                     | 0.44              |
| 1:AA:1175:G:O2'    | 1:AA:1176:A:C5'     | 2.39                     | 0.44              |
| 1:AA:189(C):C:H2'  | 1:AA:189(D):C:O4'   | 2.17                     | 0.44              |
| 1:AA:492:G:C2'     | 1:AA:493:G:O5'      | 2.64                     | 0.44              |
| 1:AA:814:A:H2'     | 1:AA:816:A:H5''     | 1.98                     | 0.44              |
| 1:AA:875:C:O2'     | 8:AH:14:ARG:HD2     | 2.17                     | 0.44              |
| 1:AA:976:G:H5'     | 1:AA:1358:U:O2'     | 2.18                     | 0.44              |
| 2:AB:93:VAL:HG11   | 2:AB:97:TRP:CD1     | 2.52                     | 0.44              |
| 3:AC:72:LYS:HG3    | 3:AC:72:LYS:O       | 2.16                     | 0.44              |
| 4:AD:102:ASP:OD1   | 4:AD:103:ASN:N      | 2.44                     | 0.44              |
| 4:AD:204:ILE:HD13  | 5:AE:97:GLY:O       | 2.17                     | 0.44              |
| 24:AY:391:GLY:C    | 24:AY:393:ASP:H     | 2.21                     | 0.44              |
| 24:AY:556:ILE:HG13 | 24:AY:558:PHE:HD1   | 1.83                     | 0.44              |
| 27:B2:46:GLN:HE21  | 27:B2:48:HIS:CE1    | 2.36                     | 0.44              |
| 29:B4:12:ALA:C     | 29:B4:13:ARG:HG2    | 2.36                     | 0.44              |
| 33:B8:21:LYS:HD3   | 33:B8:48:PHE:CE1    | 2.52                     | 0.44              |
| 35:BA:109:G:H2'    | 35:BA:110:G:O5'     | 2.18                     | 0.44              |
| 35:BA:1475:G:H2'   | 35:BA:1476:C:H6     | 1.82                     | 0.44              |
| 35:BA:1591:G:H8    | 35:BA:1591:G:C5'    | 2.30                     | 0.44              |
| 35:BA:1967:C:H2'   | 35:BA:1968:G:H5'    | 1.99                     | 0.44              |
| 35:BA:1268:A:C2    | 35:BA:2013:A:C4     | 3.05                     | 0.44              |
| 35:BA:2126:A:O2'   | 35:BA:2127:G:H5''   | 2.17                     | 0.44              |
| 35:BA:2307:G:H21   | 35:BA:2308:G:H5'    | 1.82                     | 0.44              |
| 35:BA:2300:G:N2    | 35:BA:2317:C:H1'    | 2.32                     | 0.44              |
| 35:BA:2334:G:H4'   | 35:BA:2335:A:OP2    | 2.16                     | 0.44              |
| 35:BA:466:A:C2'    | 35:BA:467:G:H5'     | 2.47                     | 0.44              |
| 35:BA:566:U:H2'    | 35:BA:567:A:O4'     | 2.17                     | 0.44              |
| 35:BA:614(A):U:H4' | 35:BA:614(B):G:H5'' | 1.97                     | 0.44              |
| 37:BC:30:VAL:CG2   | 37:BC:31:LYS:N      | 2.78                     | 0.44              |
| 38:BD:46:GLN:N     | 38:BD:46:GLN:OE1    | 2.50                     | 0.44              |
| 39:BE:181:LEU:HD21 | 52:BT:7:ILE:CG2     | 2.46                     | 0.44              |
| 39:BE:55:ASN:HA    | 39:BE:55:ASN:HD22   | 1.51                     | 0.44              |
| 39:BE:3:GLY:HA3    | 39:BE:81:ILE:HD12   | 1.99                     | 0.44              |
| 40:BF:117:ARG:HD3  | 40:BF:117:ARG:HA    | 1.69                     | 0.44              |
| 40:BF:4:VAL:HA     | 40:BF:19:GLU:HB3    | 1.98                     | 0.44              |
| 41:BG:137:GLU:O    | 41:BG:138:GLN:HG2   | 2.17                     | 0.44              |
| 41:BG:78:SER:OG    | 41:BG:79:ASN:N      | 2.50                     | 0.44              |
| 41:BG:5:VAL:HB     | 41:BG:8:LYS:HB2     | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BH:7:LEU:HD23   | 42:BH:7:LEU:H      | 1.82                     | 0.44              |
| 47:BO:47:ILE:HG12  | 47:BO:48:PRO:HD2   | 1.99                     | 0.44              |
| 48:BP:79:ARG:N     | 48:BP:110:TYR:HD2  | 2.15                     | 0.44              |
| 49:BQ:37:LEU:HD11  | 49:BQ:130:LYS:HB2  | 1.97                     | 0.44              |
| 35:BA:1278:A:H4'   | 50:BR:34:ILE:HD12  | 1.98                     | 0.44              |
| 51:BS:97:ARG:HG3   | 51:BS:97:ARG:H     | 1.52                     | 0.44              |
| 54:BV:1:MET:O      | 54:BV:2:PHE:CB     | 2.52                     | 0.44              |
| 54:BV:39:LEU:HD12  | 54:BV:47:VAL:HG21  | 1.99                     | 0.44              |
| 57:BY:7:VAL:CB     | 57:BY:8:LYS:NZ     | 2.70                     | 0.44              |
| 49:BQ:20:ALA:HB1   | 58:BZ:78:LYS:HB3   | 1.98                     | 0.44              |
| 1:AA:1080:A:O5'    | 1:AA:1080:A:H8     | 1.99                     | 0.44              |
| 1:AA:1202:G:H2'    | 1:AA:1203:C:H5'    | 1.99                     | 0.44              |
| 1:AA:1236:A:H2'    | 1:AA:1237:C:C6     | 2.53                     | 0.44              |
| 1:AA:1244:C:H2'    | 1:AA:1245:A:C8     | 2.52                     | 0.44              |
| 1:AA:1501:C:C4     | 1:AA:1504:G:C5     | 3.04                     | 0.44              |
| 1:AA:647:C:O2'     | 1:AA:648:A:H5'     | 2.16                     | 0.44              |
| 1:AA:690:G:C5      | 1:AA:691:G:C5      | 3.05                     | 0.44              |
| 1:AA:694:A:OP1     | 11:AK:53:SER:HB3   | 2.17                     | 0.44              |
| 1:AA:692:U:H2'     | 1:AA:694:A:OP2     | 2.17                     | 0.44              |
| 1:AA:748:C:O2'     | 1:AA:749:C:OP2     | 2.35                     | 0.44              |
| 3:AC:129:ALA:O     | 3:AC:131:ARG:N     | 2.50                     | 0.44              |
| 4:AD:126:ILE:N     | 4:AD:126:ILE:CD1   | 2.81                     | 0.44              |
| 4:AD:34:GLU:O      | 4:AD:35:ARG:HG3    | 2.16                     | 0.44              |
| 6:AF:44:GLY:O      | 6:AF:46:ARG:HG3    | 2.16                     | 0.44              |
| 7:AG:22:LEU:C      | 7:AG:24:THR:H      | 2.18                     | 0.44              |
| 9:AI:117:HIS:O     | 9:AI:118:LYS:CB    | 2.65                     | 0.44              |
| 9:AI:53:VAL:HG11   | 9:AI:95:LYS:HE2    | 1.95                     | 0.44              |
| 10:AJ:16:LEU:HD12  | 10:AJ:70:ARG:HG3   | 1.99                     | 0.44              |
| 12:AL:117:ARG:CZ   | 12:AL:124:LYS:HA   | 2.47                     | 0.44              |
| 14:AN:59:ALA:O     | 14:AN:60:SER:CB    | 2.65                     | 0.44              |
| 19:AS:41:VAL:HA    | 19:AS:42:PRO:HD2   | 1.86                     | 0.44              |
| 24:AY:229:LEU:O    | 24:AY:231:TYR:N    | 2.50                     | 0.44              |
| 24:AY:424:LEU:HB2  | 24:AY:472:VAL:HG11 | 2.00                     | 0.44              |
| 24:AY:555:LEU:HD13 | 24:AY:601:ILE:HG13 | 1.99                     | 0.44              |
| 25:B0:11:ARG:CD    | 25:B0:11:ARG:N     | 2.81                     | 0.44              |
| 25:B0:66:VAL:HG13  | 25:B0:67:VAL:H     | 1.82                     | 0.44              |
| 26:B1:58:ILE:HD11  | 26:B1:90:ILE:CG2   | 2.48                     | 0.44              |
| 27:B2:38:GLN:HB3   | 27:B2:44:LEU:HB3   | 1.99                     | 0.44              |
| 29:B4:57:GLU:HB2   | 29:B4:58:ARG:HD2   | 1.99                     | 0.44              |
| 29:B4:68:ARG:O     | 29:B4:71:ARG:HG2   | 2.17                     | 0.44              |
| 33:B8:38:GLY:O     | 33:B8:42:ARG:N     | 2.48                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1006:C:O2    | 46:BN:106:MET:HG2  | 2.17                     | 0.44              |
| 35:BA:104:U:C5     | 35:BA:105:C:C5     | 3.05                     | 0.44              |
| 35:BA:1106:G:H2'   | 35:BA:1107:G:C8    | 2.52                     | 0.44              |
| 35:BA:1642:G:O2'   | 35:BA:1643:G:C5'   | 2.65                     | 0.44              |
| 35:BA:1801:G:H3'   | 35:BA:1802:A:H5'   | 1.98                     | 0.44              |
| 35:BA:2134:A:O2'   | 35:BA:2135:A:H5'   | 2.16                     | 0.44              |
| 35:BA:2308:G:N7    | 35:BA:2310:A:H5'   | 2.32                     | 0.44              |
| 35:BA:2593:U:H2'   | 35:BA:2594:C:H6    | 1.83                     | 0.44              |
| 35:BA:2606:C:C3'   | 35:BA:2607:G:C5'   | 2.94                     | 0.44              |
| 35:BA:2630:G:H1'   | 35:BA:2894:G:N9    | 2.32                     | 0.44              |
| 35:BA:304:G:O2'    | 35:BA:305:U:H5'    | 2.16                     | 0.44              |
| 35:BA:310:A:OP1    | 57:BY:18:GLY:HA2   | 2.16                     | 0.44              |
| 35:BA:49:A:C5      | 35:BA:177:G:C6     | 3.05                     | 0.44              |
| 35:BA:623:G:H2'    | 35:BA:624:C:C6     | 2.52                     | 0.44              |
| 35:BA:958:U:O2'    | 35:BA:959:A:OP2    | 2.30                     | 0.44              |
| 39:BE:33:VAL:O     | 39:BE:33:VAL:HG13  | 2.17                     | 0.44              |
| 41:BG:16:ARG:N     | 41:BG:17:PRO:HD2   | 2.32                     | 0.44              |
| 41:BG:25:TYR:CE2   | 41:BG:26:GLN:OE1   | 2.70                     | 0.44              |
| 41:BG:80:PHE:O     | 41:BG:81:LYS:CB    | 2.65                     | 0.44              |
| 41:BG:87:PRO:C     | 41:BG:88:ILE:HG13  | 2.37                     | 0.44              |
| 42:BH:158:HIS:HB2  | 42:BH:159:GLU:H    | 1.63                     | 0.44              |
| 45:BL:113:UNK:O    | 45:BL:115:UNK:N    | 2.50                     | 0.44              |
| 46:BN:15:LEU:C     | 46:BN:15:LEU:HD13  | 2.38                     | 0.44              |
| 48:BP:114:ILE:O    | 48:BP:115:LEU:HB3  | 2.18                     | 0.44              |
| 48:BP:85:LEU:HD23  | 48:BP:86:LYS:H     | 1.78                     | 0.44              |
| 52:BT:41:ARG:HD3   | 52:BT:41:ARG:O     | 2.17                     | 0.44              |
| 30:B5:39:MET:HB2   | 55:BW:34:ASN:ND2   | 2.32                     | 0.44              |
| 58:BZ:128:VAL:HG11 | 58:BZ:133:ILE:HD13 | 1.98                     | 0.44              |
| 58:BZ:5:LEU:HD13   | 58:BZ:6:LYS:N      | 2.32                     | 0.44              |
| 1:AA:1342:C:H2'    | 1:AA:1343:G:C8     | 2.52                     | 0.44              |
| 1:AA:1367:C:H2'    | 1:AA:1368:G:O5'    | 2.16                     | 0.44              |
| 1:AA:1384:C:H2'    | 1:AA:1385:G:H8     | 1.83                     | 0.44              |
| 1:AA:226:G:C2'     | 1:AA:227:G:H5'     | 2.47                     | 0.44              |
| 1:AA:324:G:O5'     | 1:AA:324:G:H8      | 2.00                     | 0.44              |
| 1:AA:488:C:N4      | 1:AA:489:C:N4      | 2.66                     | 0.44              |
| 1:AA:698:G:H2'     | 1:AA:699:C:H6      | 1.79                     | 0.44              |
| 1:AA:861:G:C2'     | 1:AA:862:C:H5'     | 2.46                     | 0.44              |
| 2:AB:82:ARG:NH1    | 2:AB:82:ARG:CG     | 2.80                     | 0.44              |
| 3:AC:129:ALA:HB1   | 3:AC:133:ALA:N     | 2.31                     | 0.44              |
| 1:AA:413:G:O6      | 4:AD:35:ARG:HD2    | 2.17                     | 0.44              |
| 9:AI:42:ARG:NH2    | 9:AI:75:ASP:OD1    | 2.51                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:AM:40:ASN:HB3   | 13:AM:43:THR:CG2    | 2.47                     | 0.44              |
| 19:AS:32:LYS:CA    | 19:AS:50:ALA:HB3    | 2.47                     | 0.44              |
| 24:AY:128:TYR:O    | 24:AY:129:LYS:C     | 2.54                     | 0.44              |
| 24:AY:510:VAL:HG13 | 24:AY:567:LEU:HD11  | 1.98                     | 0.44              |
| 25:B0:50:ASN:O     | 25:B0:62:LEU:HD23   | 2.15                     | 0.44              |
| 35:BA:1287:A:C5    | 35:BA:1288:U:C4     | 3.05                     | 0.44              |
| 35:BA:1345:C:H42   | 35:BA:1601:G:H1     | 1.64                     | 0.44              |
| 35:BA:1799:G:H8    | 38:BD:181:GLU:CD    | 2.20                     | 0.44              |
| 35:BA:2008:C:O2'   | 35:BA:2009:G:H5'    | 2.17                     | 0.44              |
| 35:BA:2065:C:H2'   | 35:BA:2066:C:C6     | 2.52                     | 0.44              |
| 35:BA:2128:C:O2'   | 35:BA:2129:C:P      | 2.76                     | 0.44              |
| 35:BA:2410:G:C2    | 35:BA:2411:A:H1'    | 2.52                     | 0.44              |
| 35:BA:2581:G:C6    | 35:BA:2610:C:C4     | 3.05                     | 0.44              |
| 35:BA:524:U:H2'    | 35:BA:525:U:C6      | 2.52                     | 0.44              |
| 35:BA:654(M):C:H2' | 35:BA:654(N):G:N7   | 2.33                     | 0.44              |
| 32:B7:11:LYS:HE2   | 35:BA:686:G:H5''    | 1.99                     | 0.44              |
| 35:BA:1902:C:H4'   | 38:BD:244:ARG:HB2   | 2.00                     | 0.44              |
| 38:BD:248:SER:CB   | 38:BD:249:PRO:CD    | 2.89                     | 0.44              |
| 40:BF:9:ILE:CB     | 40:BF:14:PRO:HA     | 2.47                     | 0.44              |
| 40:BF:162:LEU:N    | 40:BF:162:LEU:HD12  | 2.31                     | 0.44              |
| 40:BF:80:ALA:HB1   | 40:BF:81:PRO:CD     | 2.44                     | 0.44              |
| 41:BG:110:ALA:O    | 41:BG:111:LEU:C     | 2.56                     | 0.44              |
| 41:BG:136:ARG:O    | 41:BG:138:GLN:N     | 2.50                     | 0.44              |
| 41:BG:144:ILE:CG2  | 41:BG:145:THR:N     | 2.80                     | 0.44              |
| 42:BH:158:HIS:N    | 42:BH:158:HIS:CD2   | 2.85                     | 0.44              |
| 42:BH:61:HIS:O     | 42:BH:62:LYS:C      | 2.55                     | 0.44              |
| 44:BK:122:UNK:O    | 44:BK:124:UNK:N     | 2.50                     | 0.44              |
| 46:BN:55:VAL:HG22  | 46:BN:56:ASN:N      | 2.33                     | 0.44              |
| 46:BN:65:LYS:O     | 46:BN:69:GLN:HB2    | 2.17                     | 0.44              |
| 48:BP:138:LEU:HD23 | 48:BP:143:GLY:O     | 2.17                     | 0.44              |
| 54:BV:19:LYS:NZ    | 54:BV:20:LEU:HB2    | 2.28                     | 0.44              |
| 54:BV:34:GLU:O     | 54:BV:36:PRO:CD     | 2.65                     | 0.44              |
| 58:BZ:7:ALA:C      | 58:BZ:8:TYR:CD1     | 2.91                     | 0.44              |
| 1:AA:1001:A:O2'    | 1:AA:1001(A):G:H5'' | 2.17                     | 0.44              |
| 1:AA:1027:C:C3'    | 1:AA:1028:C:H5''    | 2.41                     | 0.44              |
| 1:AA:173:U:H5'     | 1:AA:197:A:H5'      | 1.95                     | 0.44              |
| 1:AA:590:C:OP1     | 8:AH:30:ARG:HB2     | 2.18                     | 0.44              |
| 1:AA:884:U:H4'     | 1:AA:885:G:H5''     | 2.00                     | 0.44              |
| 1:AA:995:C:O4'     | 14:AN:8:GLU:OE1     | 2.35                     | 0.44              |
| 2:AB:145:LEU:CD2   | 2:AB:149:LEU:HD21   | 2.45                     | 0.44              |
| 2:AB:155:LEU:HD23  | 2:AB:155:LEU:HA     | 1.78                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:195:ASP:O     | 8:AH:68:ARG:NH2    | 2.50                     | 0.44              |
| 6:AF:53:ALA:O      | 6:AF:54:LYS:HB2    | 2.17                     | 0.44              |
| 7:AG:73:MET:HA     | 7:AG:91:VAL:HG23   | 1.99                     | 0.44              |
| 16:AP:53:VAL:HG23  | 16:AP:54:GLU:N     | 2.32                     | 0.44              |
| 24:AY:348:ARG:CG   | 24:AY:348:ARG:NH1  | 2.80                     | 0.44              |
| 27:B2:35:LEU:C     | 27:B2:37:PHE:H     | 2.21                     | 0.44              |
| 27:B2:45:SER:O     | 27:B2:47:ASN:N     | 2.45                     | 0.44              |
| 27:B2:55:ARG:NH1   | 27:B2:55:ARG:HG3   | 2.26                     | 0.44              |
| 28:B3:52:HIS:C     | 28:B3:53:LEU:HG    | 2.37                     | 0.44              |
| 29:B4:38:LYS:O     | 29:B4:40:HIS:N     | 2.50                     | 0.44              |
| 29:B4:62:ARG:O     | 29:B4:63:TYR:HB2   | 2.18                     | 0.44              |
| 31:B6:36:LEU:CD1   | 31:B6:50:ARG:NH1   | 2.81                     | 0.44              |
| 32:B7:34:ARG:HB2   | 32:B7:42:LEU:CD2   | 2.47                     | 0.44              |
| 35:BA:1165:U:O2'   | 35:BA:1166:C:H5'   | 2.18                     | 0.44              |
| 35:BA:1224:C:N4    | 35:BA:1225:G:C6    | 2.85                     | 0.44              |
| 35:BA:1379:A:N3    | 35:BA:1379:A:O5'   | 2.51                     | 0.44              |
| 35:BA:1413:G:H2'   | 35:BA:1414:G:O5'   | 2.17                     | 0.44              |
| 35:BA:1503:U:O2'   | 35:BA:1504:C:H5'   | 2.18                     | 0.44              |
| 35:BA:1925:C:C4    | 35:BA:1926:U:H5    | 2.36                     | 0.44              |
| 35:BA:1994:C:C6    | 35:BA:1994:C:O5'   | 2.62                     | 0.44              |
| 35:BA:2025:C:H2'   | 35:BA:2026:C:C6    | 2.52                     | 0.44              |
| 35:BA:2128:C:H1'   | 35:BA:2129:C:C5'   | 2.47                     | 0.44              |
| 35:BA:2283:C:H2'   | 35:BA:2284:C:O4'   | 2.17                     | 0.44              |
| 35:BA:2537:U:H2'   | 35:BA:2538:C:C6    | 2.52                     | 0.44              |
| 35:BA:2585:U:O2'   | 35:BA:2586:C:OP2   | 2.33                     | 0.44              |
| 35:BA:449:A:H4'    | 53:BU:3:ARG:NH2    | 2.32                     | 0.44              |
| 35:BA:461:C:C3'    | 35:BA:462:C:H5'    | 2.47                     | 0.44              |
| 35:BA:651:G:C6     | 35:BA:652:C:C4     | 3.05                     | 0.44              |
| 35:BA:833:U:H5'    | 48:BP:48:PRO:HB2   | 1.99                     | 0.44              |
| 35:BA:839:U:H2'    | 35:BA:840:C:C6     | 2.53                     | 0.44              |
| 36:BB:105:A:H4'    | 58:BZ:89:PHE:CE1   | 2.53                     | 0.44              |
| 36:BB:67:G:O2'     | 36:BB:68:C:C6      | 2.67                     | 0.44              |
| 36:BB:81:G:N3      | 36:BB:81:G:H5'     | 2.32                     | 0.44              |
| 37:BC:88:GLU:HA    | 37:BC:92:ALA:HB3   | 1.98                     | 0.44              |
| 38:BD:25:THR:C     | 38:BD:27:THR:H     | 2.19                     | 0.44              |
| 39:BE:14:ILE:HD11  | 39:BE:173:VAL:CG1  | 2.47                     | 0.44              |
| 39:BE:87:GLU:H     | 39:BE:87:GLU:HG3   | 1.65                     | 0.44              |
| 42:BH:121:ILE:HD11 | 42:BH:140:LYS:HB3  | 2.00                     | 0.44              |
| 46:BN:104:LYS:C    | 46:BN:106:MET:H    | 2.20                     | 0.44              |
| 47:BO:114:ILE:N    | 47:BO:114:ILE:HD12 | 2.32                     | 0.44              |
| 49:BQ:58:PHE:HB3   | 49:BQ:113:GLN:NE2  | 2.32                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:BR:34:ILE:HD13 | 50:BR:34:ILE:HA   | 1.77                     | 0.44              |
| 51:BS:106:ARG:CD  | 51:BS:108:GLY:HA3 | 2.48                     | 0.44              |
| 51:BS:15:ARG:HH12 | 51:BS:18:ILE:HD11 | 1.81                     | 0.44              |
| 35:BA:2875:C:O2'  | 52:BT:3:ARG:HD3   | 2.17                     | 0.44              |
| 52:BT:95:ARG:CB   | 52:BT:95:ARG:NH1  | 2.79                     | 0.44              |
| 54:BV:18:LEU:C    | 54:BV:18:LEU:CD2  | 2.85                     | 0.44              |
| 57:BY:51:VAL:O    | 57:BY:51:VAL:HG12 | 2.18                     | 0.44              |
| 58:BZ:29:TYR:HB3  | 58:BZ:34:ASN:HD22 | 1.81                     | 0.44              |
| 1:AA:1050:G:O2'   | 1:AA:1051:C:H5'   | 2.18                     | 0.44              |
| 1:AA:1063:C:H3'   | 1:AA:1064:G:H2'   | 2.00                     | 0.44              |
| 1:AA:1079:G:C6    | 1:AA:1080:A:N6    | 2.85                     | 0.44              |
| 1:AA:1177:G:OP2   | 9:AI:97:LYS:NZ    | 2.33                     | 0.44              |
| 1:AA:1181:G:O2'   | 1:AA:1184:G:H5'   | 2.17                     | 0.44              |
| 1:AA:1270:C:C2'   | 1:AA:1271:G:H5'   | 2.47                     | 0.44              |
| 1:AA:1270:C:O2'   | 1:AA:1271:G:H5'   | 2.17                     | 0.44              |
| 1:AA:1328:C:O2'   | 1:AA:1329:A:H5'   | 2.18                     | 0.44              |
| 1:AA:1438:G:H2'   | 1:AA:1439:C:H6    | 1.82                     | 0.44              |
| 1:AA:198:G:C6     | 1:AA:220:G:N3     | 2.86                     | 0.44              |
| 1:AA:345:C:OP2    | 1:AA:345:C:H6     | 2.00                     | 0.44              |
| 1:AA:49:U:N3      | 1:AA:361:G:N2     | 2.66                     | 0.44              |
| 1:AA:507:C:H2'    | 1:AA:508:C:OP1    | 2.18                     | 0.44              |
| 1:AA:555:C:C2     | 1:AA:556:C:C4     | 3.06                     | 0.44              |
| 1:AA:590:C:H2'    | 1:AA:591:U:C6     | 2.53                     | 0.44              |
| 1:AA:773:G:C2     | 1:AA:774:G:N7     | 2.86                     | 0.44              |
| 4:AD:3:ARG:HE     | 4:AD:5:ILE:HG13   | 1.82                     | 0.44              |
| 13:AM:67:GLU:OE2  | 13:AM:71:ARG:NH2  | 2.43                     | 0.44              |
| 14:AN:31:ARG:O    | 14:AN:32:SER:HB2  | 2.18                     | 0.44              |
| 19:AS:60:VAL:HG22 | 19:AS:62:ILE:H    | 1.82                     | 0.44              |
| 20:AT:96:GLY:O    | 20:AT:97:ALA:CB   | 2.65                     | 0.44              |
| 22:AV:73:A:C3'    | 22:AV:74:C:H5'    | 2.48                     | 0.44              |
| 27:B2:16:LEU:HB3  | 27:B2:20:GLU:HB3  | 1.98                     | 0.44              |
| 27:B2:9:GLN:O     | 27:B2:10:LEU:C    | 2.56                     | 0.44              |
| 31:B6:9:LEU:HD11  | 31:B6:11:LEU:HD12 | 2.00                     | 0.44              |
| 35:BA:1063:G:N2   | 35:BA:1074:G:H1   | 2.16                     | 0.44              |
| 35:BA:1299:G:H4'  | 35:BA:1301:A:C4   | 2.52                     | 0.44              |
| 35:BA:1301:A:C8   | 35:BA:1303:G:C8   | 3.05                     | 0.44              |
| 35:BA:1595:G:C2   | 35:BA:1596:A:C8   | 3.06                     | 0.44              |
| 35:BA:1854:A:H2'  | 35:BA:1855:G:O4'  | 2.17                     | 0.44              |
| 35:BA:1794:U:H1'  | 35:BA:1900:A:C2   | 2.53                     | 0.44              |
| 35:BA:1794:U:H1'  | 35:BA:1900:A:N3   | 2.32                     | 0.44              |
| 35:BA:2556:C:H2'  | 35:BA:2557:G:O4'  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:381:G:O2'   | 35:BA:382:G:H5'    | 2.18                     | 0.44              |
| 35:BA:445:C:O2'   | 35:BA:446:G:H5'    | 2.18                     | 0.44              |
| 35:BA:548:A:H2'   | 35:BA:549:G:C5'    | 2.47                     | 0.44              |
| 35:BA:747:U:O4'   | 35:BA:747:U:O2     | 2.35                     | 0.44              |
| 35:BA:826:U:H4'   | 48:BP:55:ARG:HB2   | 1.99                     | 0.44              |
| 37:BC:118:PRO:HB2 | 37:BC:121:MET:H    | 1.82                     | 0.44              |
| 35:BA:2169:A:C4'  | 37:BC:130:ARG:HH21 | 2.30                     | 0.44              |
| 37:BC:77:ALA:O    | 37:BC:78:ILE:HD13  | 2.17                     | 0.44              |
| 39:BE:53:PRO:O    | 39:BE:75:VAL:HG23  | 2.18                     | 0.44              |
| 39:BE:8:LYS:NZ    | 39:BE:188:VAL:HG13 | 2.31                     | 0.44              |
| 40:BF:84:VAL:C    | 40:BF:86:GLY:H     | 2.19                     | 0.44              |
| 42:BH:109:PHE:CZ  | 42:BH:152:ARG:HD2  | 2.51                     | 0.44              |
| 42:BH:167:GLU:N   | 42:BH:168:PRO:CD   | 2.81                     | 0.44              |
| 42:BH:5:GLY:HA2   | 42:BH:69:ARG:HB2   | 2.00                     | 0.44              |
| 44:BK:111:UNK:O   | 44:BK:112:UNK:C    | 2.65                     | 0.44              |
| 50:BR:70:LEU:HD13 | 50:BR:75:LEU:HD12  | 1.98                     | 0.44              |
| 50:BR:79:LEU:C    | 50:BR:79:LEU:HD13  | 2.38                     | 0.44              |
| 54:BV:35:LEU:C    | 54:BV:37:VAL:N     | 2.71                     | 0.44              |
| 54:BV:69:LYS:HA   | 54:BV:87:HIS:O     | 2.17                     | 0.44              |
| 58:BZ:46:LYS:C    | 58:BZ:46:LYS:HD2   | 2.38                     | 0.44              |
| 1:AA:109:A:H3'    | 1:AA:110:C:C5'     | 2.47                     | 0.44              |
| 1:AA:312:C:C2'    | 1:AA:313:A:O5'     | 2.66                     | 0.44              |
| 1:AA:434:U:H2'    | 1:AA:435:C:O4'     | 2.18                     | 0.44              |
| 1:AA:514:C:O2'    | 1:AA:515:G:H5'     | 2.17                     | 0.44              |
| 1:AA:19:C:H4'     | 1:AA:864:A:O4'     | 2.18                     | 0.44              |
| 1:AA:960:U:O2     | 1:AA:960:U:H2'     | 2.17                     | 0.44              |
| 2:AB:124:SER:HB2  | 2:AB:125:PRO:HD2   | 1.99                     | 0.44              |
| 3:AC:36:ASP:OD1   | 3:AC:57:ILE:HG21   | 2.17                     | 0.44              |
| 3:AC:64:VAL:CB    | 3:AC:99:VAL:HG12   | 2.47                     | 0.44              |
| 7:AG:36:LYS:O     | 7:AG:37:ASN:CB     | 2.64                     | 0.44              |
| 8:AH:100:ILE:HA   | 8:AH:101:PRO:HD3   | 1.82                     | 0.44              |
| 9:AI:23:ASN:HB2   | 9:AI:24:GLY:H      | 1.52                     | 0.44              |
| 10:AJ:50:ILE:CD1  | 10:AJ:57:LYS:HD3   | 2.46                     | 0.44              |
| 14:AN:55:GLY:O    | 14:AN:56:VAL:HB    | 2.18                     | 0.44              |
| 15:AO:56:LEU:HD13 | 15:AO:60:VAL:HG23  | 1.99                     | 0.44              |
| 18:AR:44:LEU:HD22 | 18:AR:79:LEU:HD22  | 1.99                     | 0.44              |
| 19:AS:40:ILE:CG2  | 19:AS:69:HIS:H     | 2.29                     | 0.44              |
| 19:AS:86:GLU:O    | 19:AS:87:ALA:CB    | 2.65                     | 0.44              |
| 22:AV:39:U:C2     | 22:AV:40:C:C5      | 3.06                     | 0.44              |
| 7:AG:81:GLY:HA3   | 23:AX:12:A:O3'     | 2.17                     | 0.44              |
| 24:AY:20:HIS:CG   | 24:AY:21:ILE:N     | 2.86                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:AY:238:THR:C   | 24:AY:240:GLU:N   | 2.70                     | 0.44              |
| 26:B1:11:ARG:CG   | 26:B1:11:ARG:HH11 | 2.25                     | 0.44              |
| 29:B4:56:VAL:HG23 | 29:B4:60:GLN:CG   | 2.44                     | 0.44              |
| 30:B5:44:THR:HG21 | 50:BR:101:ALA:CB  | 2.46                     | 0.44              |
| 31:B6:19:ARG:O    | 31:B6:20:ASN:O    | 2.35                     | 0.44              |
| 35:BA:1032:A:H2   | 35:BA:1122:G:H22  | 1.66                     | 0.44              |
| 35:BA:1301:A:C2'  | 35:BA:1302:A:C2'  | 2.93                     | 0.44              |
| 35:BA:1590:U:C3'  | 35:BA:1591:G:H5'' | 2.44                     | 0.44              |
| 35:BA:2358:G:H2'  | 35:BA:2359:C:C5'  | 2.39                     | 0.44              |
| 35:BA:2515:C:O2'  | 35:BA:2516:G:H5'  | 2.16                     | 0.44              |
| 35:BA:2656:U:C2'  | 35:BA:2657:A:H5'' | 2.45                     | 0.44              |
| 35:BA:265:A:H5'   | 35:BA:265:A:N3    | 2.33                     | 0.44              |
| 35:BA:414:C:H2'   | 35:BA:415:A:C8    | 2.53                     | 0.44              |
| 35:BA:47:C:N3     | 35:BA:179:G:C2    | 2.86                     | 0.44              |
| 35:BA:880:G:C3'   | 35:BA:881:G:H5''  | 2.46                     | 0.44              |
| 35:BA:967:C:C6    | 35:BA:967:C:O5'   | 2.66                     | 0.44              |
| 39:BE:144:ARG:HB3 | 39:BE:145:LYS:H   | 1.46                     | 0.44              |
| 39:BE:1:MET:O     | 39:BE:2:LYS:C     | 2.55                     | 0.44              |
| 40:BF:6:VAL:CG1   | 40:BF:7:TYR:N     | 2.66                     | 0.44              |
| 41:BG:57:ALA:N    | 41:BG:90:LEU:HD21 | 2.33                     | 0.44              |
| 45:BL:97:UNK:O    | 45:BL:98:UNK:CB   | 2.65                     | 0.44              |
| 48:BP:62:LEU:O    | 48:BP:62:LEU:HG   | 2.18                     | 0.44              |
| 50:BR:50:HIS:CD2  | 50:BR:54:LEU:HD11 | 2.53                     | 0.44              |
| 52:BT:117:ASP:OD1 | 52:BT:119:LYS:HB3 | 2.17                     | 0.44              |
| 53:BU:66:ASN:ND2  | 53:BU:70:ARG:HE   | 2.15                     | 0.44              |
| 57:BY:44:ILE:CG2  | 57:BY:45:VAL:N    | 2.78                     | 0.44              |
| 1:AA:105:G:C4     | 1:AA:106:C:C4     | 3.06                     | 0.44              |
| 1:AA:1258:G:H2'   | 1:AA:1259:C:C6    | 2.53                     | 0.44              |
| 1:AA:1268:A:C8    | 1:AA:1326:C:O2'   | 2.70                     | 0.44              |
| 1:AA:1279:A:O2'   | 1:AA:1281:U:H5''  | 2.18                     | 0.44              |
| 1:AA:1452:C:O2'   | 1:AA:1456:G:P     | 2.75                     | 0.44              |
| 1:AA:173:U:H5'    | 1:AA:197:A:C4'    | 2.48                     | 0.44              |
| 1:AA:262:A:H2'    | 1:AA:263:A:C8     | 2.53                     | 0.44              |
| 1:AA:620:C:H2'    | 1:AA:621:A:O4'    | 2.18                     | 0.44              |
| 7:AG:44:TYR:C     | 7:AG:46:ALA:N     | 2.68                     | 0.44              |
| 1:AA:973:G:C1'    | 10:AJ:55:LYS:HG2  | 2.46                     | 0.44              |
| 12:AL:43:VAL:CG1  | 12:AL:44:THR:N    | 2.81                     | 0.44              |
| 14:AN:9:LYS:HA    | 14:AN:12:ARG:NH2  | 2.33                     | 0.44              |
| 15:AO:56:LEU:HD13 | 15:AO:56:LEU:C    | 2.38                     | 0.44              |
| 19:AS:20:LEU:HD22 | 29:B4:61:ARG:HH21 | 1.82                     | 0.44              |
| 19:AS:50:ALA:HB1  | 19:AS:57:HIS:HB3  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:AS:75:ALA:O     | 19:AS:76:PRO:C     | 2.56                     | 0.44              |
| 24:AY:149:VAL:O    | 24:AY:152:THR:HG22 | 2.18                     | 0.44              |
| 24:AY:156:ARG:HH22 | 24:AY:666:ARG:CZ   | 2.29                     | 0.44              |
| 24:AY:40:HIS:HB3   | 24:AY:41:LYS:H     | 1.60                     | 0.44              |
| 24:AY:512:ILE:CD1  | 24:AY:589:ALA:HB1  | 2.47                     | 0.44              |
| 24:AY:530:VAL:HG13 | 24:AY:531:GLY:H    | 1.82                     | 0.44              |
| 27:B2:44:LEU:O     | 27:B2:44:LEU:CD1   | 2.64                     | 0.44              |
| 29:B4:7:PRO:HG2    | 29:B4:9:LEU:HD12   | 1.97                     | 0.44              |
| 34:B9:8:LYS:O      | 34:B9:25:VAL:HG21  | 2.17                     | 0.44              |
| 35:BA:1094:U:H5'   | 35:BA:1095:A:OP2   | 2.17                     | 0.44              |
| 35:BA:1204:A:H2    | 35:BA:1241:A:N1    | 2.15                     | 0.44              |
| 35:BA:121:G:H4'    | 35:BA:149:A:H5'    | 2.00                     | 0.44              |
| 35:BA:1767:C:C2'   | 35:BA:1768:U:C5'   | 2.78                     | 0.44              |
| 35:BA:1778:U:H6    | 35:BA:1778:U:O5'   | 1.99                     | 0.44              |
| 35:BA:181:A:C2     | 35:BA:435:C:C5     | 3.06                     | 0.44              |
| 35:BA:2019:A:H2'   | 35:BA:2020:A:O5'   | 2.18                     | 0.44              |
| 35:BA:528:A:C2     | 35:BA:2043:C:H4'   | 2.53                     | 0.44              |
| 35:BA:2402:C:H1'   | 35:BA:2403:C:OP2   | 2.18                     | 0.44              |
| 35:BA:2403:C:C6    | 35:BA:2403:C:O5'   | 2.71                     | 0.44              |
| 35:BA:2464:C:HO2'  | 35:BA:2465:C:P     | 2.41                     | 0.44              |
| 35:BA:2517:C:C6    | 35:BA:2542:A:C2    | 3.06                     | 0.44              |
| 35:BA:533:G:H5'    | 53:BU:24:TYR:CE1   | 2.52                     | 0.44              |
| 37:BC:55:SER:C     | 37:BC:57:GLN:N     | 2.71                     | 0.44              |
| 37:BC:7:ARG:HH22   | 37:BC:219:MET:HB2  | 1.82                     | 0.44              |
| 38:BD:244:ARG:HA   | 38:BD:245:PRO:HA   | 1.51                     | 0.44              |
| 39:BE:154:LYS:O    | 39:BE:154:LYS:CG   | 2.66                     | 0.44              |
| 39:BE:164:ARG:NH2  | 39:BE:199:ARG:NH2  | 2.65                     | 0.44              |
| 40:BF:10:PRO:O     | 40:BF:11:VAL:HG23  | 2.17                     | 0.44              |
| 40:BF:37:VAL:HG11  | 48:BP:7:ARG:HH12   | 1.81                     | 0.44              |
| 41:BG:16:ARG:HB3   | 41:BG:17:PRO:CD    | 2.48                     | 0.44              |
| 41:BG:9:ARG:CD     | 41:BG:9:ARG:H      | 2.25                     | 0.44              |
| 46:BN:51:PHE:CZ    | 46:BN:119:ARG:HD2  | 2.52                     | 0.44              |
| 46:BN:3:THR:CG2    | 46:BN:4:TYR:H      | 2.23                     | 0.44              |
| 46:BN:73:THR:HG23  | 46:BN:82:LEU:CD1   | 2.48                     | 0.44              |
| 48:BP:57:THR:C     | 48:BP:59:LEU:N     | 2.46                     | 0.44              |
| 50:BR:4:LEU:C      | 50:BR:6:SER:N      | 2.70                     | 0.44              |
| 35:BA:1217:C:OP2   | 53:BU:15:LYS:HE3   | 2.18                     | 0.44              |
| 54:BV:55:ALA:O     | 54:BV:56:SER:HB3   | 2.18                     | 0.44              |
| 55:BW:110:LYS:HA   | 55:BW:110:LYS:HD2  | 1.77                     | 0.44              |
| 55:BW:2:GLU:OE2    | 55:BW:106:ILE:HD12 | 2.17                     | 0.44              |
| 57:BY:6:HIS:N      | 57:BY:6:HIS:CD2    | 2.85                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 58:BZ:122:ARG:HH11 | 58:BZ:122:ARG:CB  | 2.30                     | 0.44              |
| 58:BZ:44:PHE:CZ    | 58:BZ:48:PHE:CD2  | 2.98                     | 0.44              |
| 1:AA:1073:U:C2'    | 1:AA:1074:G:C5'   | 2.76                     | 0.44              |
| 1:AA:1371:G:OP1    | 9:AI:12:GLU:HB2   | 2.17                     | 0.44              |
| 1:AA:363:A:H8      | 1:AA:363:A:O5'    | 2.01                     | 0.44              |
| 1:AA:498:U:O2'     | 1:AA:499:A:P      | 2.76                     | 0.44              |
| 1:AA:818:G:HO2'    | 1:AA:820:U:H6     | 1.64                     | 0.44              |
| 1:AA:961:U:C6      | 1:AA:962:C:C5     | 3.06                     | 0.44              |
| 1:AA:979:C:C3'     | 1:AA:980:C:C5'    | 2.94                     | 0.44              |
| 2:AB:165:VAL:HG23  | 2:AB:166:ASP:H    | 1.82                     | 0.44              |
| 12:AL:5:PRO:HB2    | 12:AL:9:GLN:HB2   | 1.98                     | 0.44              |
| 13:AM:39:ILE:CD1   | 13:AM:56:LEU:HB2  | 2.48                     | 0.44              |
| 13:AM:45:VAL:HA    | 13:AM:48:LEU:HG   | 1.99                     | 0.44              |
| 13:AM:70:LEU:O     | 13:AM:71:ARG:C    | 2.56                     | 0.44              |
| 14:AN:12:ARG:HB3   | 14:AN:14:PRO:CD   | 2.48                     | 0.44              |
| 12:AL:10:LEU:HB3   | 17:AQ:32:TYR:CE2  | 2.53                     | 0.44              |
| 22:AV:15:G:H5'     | 22:AV:16:C:O2     | 2.18                     | 0.44              |
| 24:AY:229:LEU:HA   | 24:AY:232:LEU:CD2 | 2.48                     | 0.44              |
| 24:AY:165:GLN:OE1  | 24:AY:259:PHE:HD2 | 2.01                     | 0.44              |
| 24:AY:587:SER:O    | 24:AY:591:LYS:HB2 | 2.17                     | 0.44              |
| 24:AY:7:TYR:CD2    | 24:AY:370:LYS:HD2 | 2.52                     | 0.44              |
| 28:B3:54:VAL:O     | 28:B3:54:VAL:HG22 | 2.17                     | 0.44              |
| 29:B4:22:ILE:HG13  | 41:BG:105:LYS:HD3 | 2.00                     | 0.44              |
| 29:B4:52:THR:O     | 29:B4:53:GLU:C    | 2.56                     | 0.44              |
| 33:B8:23:VAL:HG12  | 33:B8:46:ARG:NH1  | 2.24                     | 0.44              |
| 35:BA:1047:G:H2'   | 35:BA:1110:G:N2   | 2.33                     | 0.44              |
| 35:BA:1180:C:H2'   | 35:BA:1181:C:H5'  | 2.00                     | 0.44              |
| 35:BA:1215:G:C2'   | 35:BA:1216:G:C5'  | 2.90                     | 0.44              |
| 35:BA:1249:U:C4'   | 53:BU:4:ALA:HB3   | 2.47                     | 0.44              |
| 35:BA:1446:C:H3'   | 35:BA:1446:C:O2   | 2.18                     | 0.44              |
| 35:BA:1493:C:C2'   | 35:BA:1493:C:O2   | 2.66                     | 0.44              |
| 35:BA:181:A:C6     | 35:BA:182:A:C6    | 3.06                     | 0.44              |
| 35:BA:1982:C:C4    | 35:BA:1983:C:C4   | 3.04                     | 0.44              |
| 35:BA:1992:G:C2    | 35:BA:1997:G:C5   | 3.06                     | 0.44              |
| 35:BA:2207:G:H5''  | 35:BA:2207:G:C2   | 2.48                     | 0.44              |
| 35:BA:221:A:O2'    | 35:BA:222:A:OP2   | 2.32                     | 0.44              |
| 35:BA:2259:G:C8    | 35:BA:2427:C:C4   | 3.06                     | 0.44              |
| 35:BA:2364:C:H2'   | 35:BA:2365:G:O4'  | 2.18                     | 0.44              |
| 35:BA:2468:G:OP1   | 49:BQ:119:ARG:NH2 | 2.47                     | 0.44              |
| 35:BA:264:C:H4'    | 35:BA:428:A:C2    | 2.53                     | 0.44              |
| 35:BA:2884:U:H2'   | 35:BA:2885:C:H5'  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:327:G:O2'   | 35:BA:328:U:O5'    | 2.36                     | 0.44              |
| 35:BA:876:C:H2'   | 35:BA:877:U:O4'    | 2.18                     | 0.44              |
| 36:BB:37:C:H2'    | 36:BB:38:C:C5'     | 2.48                     | 0.44              |
| 37:BC:130:ARG:O   | 37:BC:130:ARG:HG3  | 2.17                     | 0.44              |
| 37:BC:75:VAL:CG2  | 37:BC:92:ALA:HA    | 2.47                     | 0.44              |
| 38:BD:43:ARG:HB3  | 38:BD:54:ARG:CB    | 2.43                     | 0.44              |
| 40:BF:26:ALA:C    | 40:BF:27:GLU:OE1   | 2.57                     | 0.44              |
| 42:BH:11:VAL:HG12 | 42:BH:12:PRO:O     | 2.17                     | 0.44              |
| 42:BH:85:LYS:NZ   | 42:BH:145:ALA:HA   | 2.32                     | 0.44              |
| 44:BK:6:UNK:O     | 44:BK:7:UNK:CB     | 2.64                     | 0.44              |
| 49:BQ:16:ARG:HG3  | 49:BQ:17:LEU:H     | 1.82                     | 0.44              |
| 54:BV:1:MET:HB3   | 54:BV:2:PHE:H      | 1.55                     | 0.44              |
| 54:BV:57:VAL:HG23 | 54:BV:99:ILE:HG23  | 2.00                     | 0.44              |
| 55:BW:37:ARG:NH1  | 55:BW:37:ARG:HG3   | 2.30                     | 0.44              |
| 58:BZ:118:GLN:HG2 | 58:BZ:120:ILE:HD13 | 2.00                     | 0.44              |
| 1:AA:1157:A:C1'   | 1:AA:1158:C:P      | 3.05                     | 0.44              |
| 1:AA:1280:A:O4'   | 10:AJ:41:PRO:CG    | 2.63                     | 0.44              |
| 1:AA:415:A:H2'    | 1:AA:416:G:H8      | 1.83                     | 0.44              |
| 1:AA:975:A:C4'    | 1:AA:976:G:H5''    | 2.25                     | 0.44              |
| 3:AC:167:TRP:CD1  | 3:AC:168:ALA:C     | 2.91                     | 0.44              |
| 9:AI:19:LEU:O     | 9:AI:19:LEU:HD12   | 2.18                     | 0.44              |
| 9:AI:42:ARG:HH22  | 9:AI:75:ASP:CG     | 2.21                     | 0.44              |
| 10:AJ:37:PRO:HA   | 10:AJ:71:LEU:O     | 2.18                     | 0.44              |
| 12:AL:28:LYS:O    | 12:AL:29:GLY:C     | 2.55                     | 0.44              |
| 13:AM:18:ALA:O    | 13:AM:19:LEU:C     | 2.55                     | 0.44              |
| 13:AM:49:THR:O    | 13:AM:50:GLU:C     | 2.57                     | 0.44              |
| 17:AQ:9:VAL:HG11  | 17:AQ:84:LEU:HD12  | 1.99                     | 0.44              |
| 24:AY:99:ARG:NE   | 24:AY:128:TYR:CZ   | 2.84                     | 0.44              |
| 24:AY:498:ILE:HA  | 24:AY:507:TYR:HB3  | 2.00                     | 0.44              |
| 24:AY:92:ILE:HD12 | 24:AY:96:ARG:HE    | 1.83                     | 0.44              |
| 25:B0:37:LEU:N    | 25:B0:37:LEU:HD22  | 2.27                     | 0.44              |
| 25:B0:62:LEU:CD2  | 25:B0:62:LEU:N     | 2.66                     | 0.44              |
| 19:AS:67:VAL:HG12 | 29:B4:52:THR:HG23  | 2.00                     | 0.44              |
| 29:B4:7:PRO:HB2   | 29:B4:8:LYS:H      | 1.70                     | 0.44              |
| 30:B5:45:VAL:HG13 | 30:B5:51:TYR:HB2   | 1.99                     | 0.44              |
| 35:BA:1136:G:C2   | 35:BA:1137:G:C5    | 3.06                     | 0.44              |
| 35:BA:1169:G:N2   | 35:BA:1181:C:C2    | 2.86                     | 0.44              |
| 35:BA:1464:C:O2'  | 35:BA:1528:A:H1'   | 2.18                     | 0.44              |
| 35:BA:1654:A:H1'  | 35:BA:2823:A:H5'   | 1.99                     | 0.44              |
| 35:BA:1688:U:H1'  | 35:BA:1701:A:N6    | 2.33                     | 0.44              |
| 35:BA:2037:G:H2'  | 35:BA:2038:G:C8    | 2.53                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:2202:C:H2'   | 35:BA:2203:U:C6   | 2.51                     | 0.44              |
| 35:BA:2233:U:H2'   | 35:BA:2234:G:C8   | 2.52                     | 0.44              |
| 35:BA:2287:A:C2    | 35:BA:2346:A:C2   | 3.06                     | 0.44              |
| 35:BA:256:A:O2'    | 35:BA:257:A:C5'   | 2.66                     | 0.44              |
| 35:BA:2756:U:C1'   | 35:BA:2757:A:O5'  | 2.66                     | 0.44              |
| 35:BA:478:A:N1     | 35:BA:500:G:H4'   | 2.32                     | 0.44              |
| 35:BA:49:A:N3      | 35:BA:49:A:H5'    | 2.33                     | 0.44              |
| 35:BA:807:U:OP2    | 48:BP:39:LYS:HG2  | 2.18                     | 0.44              |
| 35:BA:860:U:H2'    | 35:BA:861:A:C5'   | 2.48                     | 0.44              |
| 35:BA:940:G:H2'    | 35:BA:941:A:O4'   | 2.18                     | 0.44              |
| 37:BC:86:GLU:O     | 37:BC:87:ALA:HB3  | 2.18                     | 0.44              |
| 38:BD:3:VAL:HG13   | 38:BD:17:THR:HB   | 1.99                     | 0.44              |
| 38:BD:134:ARG:NH1  | 38:BD:188:GLU:OE2 | 2.51                     | 0.44              |
| 39:BE:33:VAL:HG23  | 39:BE:47:VAL:HG12 | 2.00                     | 0.44              |
| 39:BE:71:GLY:C     | 39:BE:73:GLU:N    | 2.71                     | 0.44              |
| 40:BF:114:VAL:HG21 | 40:BF:202:PHE:CZ  | 2.52                     | 0.44              |
| 40:BF:26:ALA:HB1   | 40:BF:27:GLU:OE1  | 2.17                     | 0.44              |
| 41:BG:117:PHE:CD2  | 41:BG:118:ARG:CD  | 2.99                     | 0.44              |
| 41:BG:38:VAL:HG12  | 41:BG:39:ILE:N    | 2.33                     | 0.44              |
| 45:BL:61:UNK:HA    | 45:BL:93:UNK:O    | 2.18                     | 0.44              |
| 48:BP:51:PHE:HD2   | 48:BP:52:GLU:O    | 1.91                     | 0.44              |
| 35:BA:2394:C:OP1   | 48:BP:63:PRO:CD   | 2.66                     | 0.44              |
| 51:BS:54:LEU:CD1   | 51:BS:57:LYS:HA   | 2.34                     | 0.44              |
| 52:BT:26:ASP:HB3   | 52:BT:89:VAL:O    | 2.18                     | 0.44              |
| 53:BU:21:ALA:O     | 53:BU:22:LYS:C    | 2.56                     | 0.44              |
| 58:BZ:39:VAL:HG21  | 58:BZ:44:PHE:HB2  | 1.99                     | 0.44              |
| 1:AA:37:U:O2'      | 1:AA:38:G:H5''    | 2.17                     | 0.43              |
| 1:AA:38:G:HO2'     | 1:AA:39:G:P       | 2.41                     | 0.43              |
| 1:AA:545:C:O2'     | 1:AA:549:C:OP1    | 2.36                     | 0.43              |
| 1:AA:936:C:H2'     | 1:AA:937:A:O5'    | 2.18                     | 0.43              |
| 3:AC:131:ARG:CB    | 3:AC:131:ARG:HH11 | 2.28                     | 0.43              |
| 3:AC:16:ARG:CD     | 3:AC:17:ASP:N     | 2.80                     | 0.43              |
| 5:AE:105:VAL:HB    | 5:AE:106:PRO:CD   | 2.48                     | 0.43              |
| 6:AF:100:ASN:O     | 18:AR:28:GLU:HG2  | 2.17                     | 0.43              |
| 7:AG:48:LYS:HG2    | 7:AG:49:ILE:H     | 1.83                     | 0.43              |
| 1:AA:1458:G:H5''   | 20:AT:31:SER:HB2  | 2.00                     | 0.43              |
| 24:AY:27:THR:O     | 24:AY:30:GLU:HB3  | 2.18                     | 0.43              |
| 24:AY:530:VAL:C    | 24:AY:532:GLY:H   | 2.20                     | 0.43              |
| 26:B1:19:GLN:HB2   | 26:B1:35:THR:HG22 | 1.99                     | 0.43              |
| 26:B1:50:ARG:H     | 26:B1:50:ARG:HG2  | 1.50                     | 0.43              |
| 27:B2:10:LEU:O     | 27:B2:14:ARG:CG   | 2.66                     | 0.43              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 28:B3:58:VAL:HG12   | 28:B3:59:VAL:N    | 2.33                     | 0.43              |
| 29:B4:48:ARG:O      | 29:B4:50:VAL:N    | 2.48                     | 0.43              |
| 29:B4:51:ASP:O      | 29:B4:53:GLU:N    | 2.50                     | 0.43              |
| 32:B7:34:ARG:CD     | 35:BA:467:G:OP2   | 2.66                     | 0.43              |
| 34:B9:7:VAL:HG12    | 34:B9:7:VAL:O     | 2.17                     | 0.43              |
| 35:BA:1086:A:N3     | 35:BA:1086:A:H3'  | 2.33                     | 0.43              |
| 35:BA:1221(A):C:C2' | 35:BA:1222:C:H5'  | 2.47                     | 0.43              |
| 35:BA:1316:U:H2'    | 35:BA:1317:A:H8   | 1.83                     | 0.43              |
| 35:BA:1449:A:H5''   | 35:BA:1449:A:H8   | 1.82                     | 0.43              |
| 35:BA:1578:U:H2'    | 35:BA:1579:A:H5'  | 1.98                     | 0.43              |
| 35:BA:1595:G:N3     | 35:BA:1596:A:C8   | 2.86                     | 0.43              |
| 35:BA:1982:C:N4     | 35:BA:1983:C:H42  | 2.13                     | 0.43              |
| 35:BA:2033:A:O2'    | 35:BA:2034:U:OP1  | 2.30                     | 0.43              |
| 35:BA:2199:A:OP2    | 35:BA:2200:C:H5   | 2.00                     | 0.43              |
| 35:BA:2203:U:O2     | 35:BA:2203:U:H2'  | 2.17                     | 0.43              |
| 35:BA:221:A:C4      | 35:BA:266:G:N7    | 2.85                     | 0.43              |
| 35:BA:2543:G:H2'    | 35:BA:2544:G:H8   | 1.83                     | 0.43              |
| 35:BA:2712:U:H5'    | 35:BA:2712:U:O2   | 2.17                     | 0.43              |
| 35:BA:47:C:N4       | 35:BA:179:G:N1    | 2.66                     | 0.43              |
| 35:BA:547:A:C6      | 35:BA:548:A:C6    | 3.06                     | 0.43              |
| 35:BA:701:G:C2'     | 35:BA:702:G:H5'   | 2.47                     | 0.43              |
| 37:BC:121:MET:HE3   | 37:BC:139:PRO:O   | 2.17                     | 0.43              |
| 37:BC:39:ASP:O      | 37:BC:178:LYS:HE3 | 2.17                     | 0.43              |
| 38:BD:221:VAL:HG22  | 38:BD:226:MET:CE  | 2.48                     | 0.43              |
| 40:BF:136:THR:HG23  | 40:BF:170:LEU:CD2 | 2.45                     | 0.43              |
| 40:BF:3:GLU:CA      | 40:BF:24:LEU:CG   | 2.95                     | 0.43              |
| 29:B4:32:TYR:HB3    | 41:BG:141:PHE:CZ  | 2.52                     | 0.43              |
| 41:BG:6:ALA:HB3     | 41:BG:105:LYS:HE3 | 1.99                     | 0.43              |
| 41:BG:37:VAL:CG2    | 41:BG:99:MET:HG3  | 2.46                     | 0.43              |
| 48:BP:96:THR:HG22   | 48:BP:126:VAL:CG2 | 2.48                     | 0.43              |
| 52:BT:30:VAL:O      | 52:BT:44:ASP:HA   | 2.18                     | 0.43              |
| 52:BT:59:THR:O      | 52:BT:77:PRO:O    | 2.36                     | 0.43              |
| 47:BO:76:ALA:HB3    | 52:BT:75:ILE:HD12 | 1.99                     | 0.43              |
| 53:BU:76:TYR:CZ     | 53:BU:80:ILE:HG13 | 2.53                     | 0.43              |
| 54:BV:76:LYS:HB2    | 54:BV:81:TYR:HB3  | 1.99                     | 0.43              |
| 1:AA:1032:G:H2'     | 1:AA:1033:G:C8    | 2.54                     | 0.43              |
| 1:AA:549:C:H2'      | 1:AA:550:G:O4'    | 2.17                     | 0.43              |
| 1:AA:684:A:H1'      | 11:AK:39:PRO:HD2  | 1.99                     | 0.43              |
| 1:AA:979:C:H3'      | 1:AA:980:C:C5'    | 2.48                     | 0.43              |
| 2:AB:19:HIS:HB3     | 2:AB:189:ASP:OD2  | 2.18                     | 0.43              |
| 2:AB:23:ARG:CG      | 2:AB:23:ARG:O     | 2.66                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AC:25:GLY:O     | 3:AC:28:GLN:N     | 2.38                     | 0.43              |
| 4:AD:108:LEU:HD12 | 4:AD:108:LEU:HA   | 1.71                     | 0.43              |
| 7:AG:87:VAL:HG23  | 7:AG:151:TYR:O    | 2.18                     | 0.43              |
| 10:AJ:49:VAL:HG22 | 10:AJ:50:ILE:O    | 2.18                     | 0.43              |
| 14:AN:12:ARG:CB   | 14:AN:14:PRO:HD2  | 2.48                     | 0.43              |
| 16:AP:52:ASP:O    | 16:AP:54:GLU:N    | 2.51                     | 0.43              |
| 24:AY:138:LYS:C   | 24:AY:140:ASP:H   | 2.21                     | 0.43              |
| 24:AY:140:ASP:OD2 | 24:AY:265:LYS:HD3 | 2.18                     | 0.43              |
| 24:AY:168:ILE:HB  | 24:AY:176:GLY:H   | 1.83                     | 0.43              |
| 24:AY:471:LYS:O   | 24:AY:471:LYS:CG  | 2.61                     | 0.43              |
| 24:AY:47:GLU:HB3  | 24:AY:52:MET:CA   | 2.47                     | 0.43              |
| 24:AY:535:PRO:O   | 24:AY:537:GLU:N   | 2.51                     | 0.43              |
| 24:AY:573:HIS:O   | 24:AY:574:GLU:HB2 | 2.18                     | 0.43              |
| 24:AY:589:ALA:O   | 24:AY:592:GLU:HG2 | 2.17                     | 0.43              |
| 29:B4:39:CYS:HB3  | 29:B4:40:HIS:H    | 1.68                     | 0.43              |
| 29:B4:56:VAL:HG13 | 29:B4:57:GLU:N    | 2.33                     | 0.43              |
| 30:B5:35:GLU:HB2  | 30:B5:49:CYS:HB3  | 2.00                     | 0.43              |
| 33:B8:27:THR:HG22 | 48:BP:62:LEU:CD2  | 2.48                     | 0.43              |
| 35:BA:16:G:N3     | 35:BA:17:G:C8     | 2.86                     | 0.43              |
| 35:BA:2354:G:N1   | 35:BA:2364:C:C4   | 2.86                     | 0.43              |
| 35:BA:239:U:H2'   | 35:BA:240:G:O4'   | 2.17                     | 0.43              |
| 35:BA:2534:A:H2'  | 35:BA:2535:G:O5'  | 2.18                     | 0.43              |
| 35:BA:2688:U:C5   | 35:BA:2720:U:OP2  | 2.71                     | 0.43              |
| 35:BA:2808:U:N3   | 35:BA:2892:A:N7   | 2.65                     | 0.43              |
| 35:BA:333:G:N3    | 35:BA:333:G:H2'   | 2.33                     | 0.43              |
| 35:BA:590:A:H2'   | 35:BA:591:C:C6    | 2.52                     | 0.43              |
| 35:BA:601:C:O2'   | 35:BA:605:C:OP1   | 2.36                     | 0.43              |
| 35:BA:900:A:N3    | 35:BA:900:A:H2'   | 2.32                     | 0.43              |
| 36:BB:8:U:C5'     | 36:BB:8:U:H6      | 2.21                     | 0.43              |
| 41:BG:20:ILE:O    | 41:BG:21:ARG:HB2  | 2.17                     | 0.43              |
| 41:BG:87:PRO:CG   | 41:BG:88:ILE:N    | 2.81                     | 0.43              |
| 45:BL:68:UNK:C    | 45:BL:70:UNK:N    | 2.79                     | 0.43              |
| 50:BR:44:LEU:HD13 | 50:BR:44:LEU:C    | 2.39                     | 0.43              |
| 51:BS:14:VAL:CG1  | 51:BS:15:ARG:H    | 2.29                     | 0.43              |
| 52:BT:125:ARG:HG2 | 52:BT:125:ARG:NH1 | 2.32                     | 0.43              |
| 52:BT:29:ARG:H    | 52:BT:45:PHE:C    | 2.21                     | 0.43              |
| 57:BY:17:SER:HB2  | 57:BY:71:LYS:HZ3  | 1.84                     | 0.43              |
| 57:BY:86:ARG:HG2  | 57:BY:87:LYS:N    | 2.33                     | 0.43              |
| 1:AA:1048:G:O2'   | 1:AA:1049:U:H3'   | 2.18                     | 0.43              |
| 1:AA:1508:G:O2'   | 1:AA:1509:C:H5'   | 2.18                     | 0.43              |
| 1:AA:152:A:H62    | 1:AA:169:C:N4     | 2.16                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:360:A:C6      | 1:AA:361:G:C6     | 3.06                     | 0.43              |
| 1:AA:491:G:C2      | 1:AA:492:G:C5     | 3.05                     | 0.43              |
| 1:AA:940:C:H2'     | 1:AA:941:G:C8     | 2.52                     | 0.43              |
| 1:AA:983:A:H1'     | 1:AA:1049:U:O2    | 2.18                     | 0.43              |
| 3:AC:164:ARG:HH11  | 3:AC:164:ARG:CG   | 2.30                     | 0.43              |
| 8:AH:42:GLU:HG3    | 8:AH:109:ILE:CD1  | 2.43                     | 0.43              |
| 9:AI:81:ILE:HG22   | 9:AI:82:ALA:N     | 2.33                     | 0.43              |
| 11:AK:105:VAL:HG23 | 11:AK:105:VAL:O   | 2.17                     | 0.43              |
| 11:AK:57:THR:CG2   | 11:AK:60:ALA:H    | 2.31                     | 0.43              |
| 1:AA:1309:G:N7     | 13:AM:99:ARG:NH2  | 2.65                     | 0.43              |
| 14:AN:25:VAL:O     | 14:AN:25:VAL:HG12 | 2.18                     | 0.43              |
| 15:AO:12:ILE:O     | 15:AO:16:ALA:HB2  | 2.18                     | 0.43              |
| 19:AS:6:LYS:CG     | 19:AS:7:LYS:N     | 2.81                     | 0.43              |
| 20:AT:57:ARG:HD2   | 20:AT:102:GLY:CA  | 2.48                     | 0.43              |
| 22:AV:11:C:H42     | 22:AV:24:G:H1     | 1.66                     | 0.43              |
| 26:B1:33:LYS:HB2   | 35:BA:2432:A:C2   | 2.53                     | 0.43              |
| 29:B4:36:CYS:C     | 29:B4:38:LYS:H    | 2.22                     | 0.43              |
| 31:B6:18:ARG:NH2   | 31:B6:44:ARG:CB   | 2.82                     | 0.43              |
| 35:BA:1068:G:H1'   | 35:BA:1069:A:OP1  | 2.18                     | 0.43              |
| 35:BA:1076:C:O5'   | 35:BA:1076:C:H6   | 2.00                     | 0.43              |
| 35:BA:1211:U:O2    | 35:BA:1211:U:O5'  | 2.35                     | 0.43              |
| 35:BA:1264:G:C2    | 35:BA:2014:A:N7   | 2.87                     | 0.43              |
| 35:BA:1378:A:C4    | 35:BA:1380:G:N7   | 2.86                     | 0.43              |
| 35:BA:1412:A:H2'   | 35:BA:1413:G:C5'  | 2.46                     | 0.43              |
| 35:BA:1458:C:O4'   | 35:BA:1459:G:C5   | 2.71                     | 0.43              |
| 35:BA:1681:G:O2'   | 35:BA:1762:A:C2'  | 2.66                     | 0.43              |
| 35:BA:1784:A:C4'   | 35:BA:1785:A:H5"  | 2.48                     | 0.43              |
| 35:BA:1784:A:H4'   | 35:BA:1785:A:O5'  | 2.18                     | 0.43              |
| 35:BA:185:U:H2'    | 35:BA:186:G:H8    | 1.84                     | 0.43              |
| 35:BA:2034:U:H2'   | 35:BA:2035:G:O5'  | 2.18                     | 0.43              |
| 35:BA:2362:G:C2'   | 35:BA:2363:C:C5'  | 2.94                     | 0.43              |
| 35:BA:2403:C:O2'   | 35:BA:2404:C:C5'  | 2.62                     | 0.43              |
| 35:BA:261:G:O2'    | 35:BA:262:A:H5'   | 2.18                     | 0.43              |
| 35:BA:630:G:H4'    | 35:BA:640:C:H4'   | 1.99                     | 0.43              |
| 35:BA:743:G:N9     | 35:BA:744:G:C8    | 2.85                     | 0.43              |
| 35:BA:910:A:H2'    | 35:BA:911:A:C8    | 2.53                     | 0.43              |
| 36:BB:111:G:H2'    | 36:BB:112:U:O4'   | 2.18                     | 0.43              |
| 38:BD:117:VAL:HG23 | 38:BD:128:GLY:C   | 2.38                     | 0.43              |
| 39:BE:132:HIS:CD2  | 39:BE:135:HIS:NE2 | 2.86                     | 0.43              |
| 35:BA:2620:C:OP1   | 39:BE:153:GLY:CA  | 2.66                     | 0.43              |
| 39:BE:56:PRO:O     | 39:BE:57:LYS:HE3  | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BF:81:PRO:HA    | 40:BF:87:GLY:O     | 2.17                     | 0.43              |
| 42:BH:137:ASP:OD2  | 42:BH:140:LYS:HE3  | 2.18                     | 0.43              |
| 43:BJ:53:UNK:C     | 43:BJ:85:LEU:HD12  | 2.46                     | 0.43              |
| 46:BN:120:LEU:HD13 | 46:BN:120:LEU:C    | 2.38                     | 0.43              |
| 48:BP:144:GLU:N    | 48:BP:145:PRO:CD   | 2.78                     | 0.43              |
| 48:BP:39:LYS:O     | 48:BP:40:SER:CB    | 2.67                     | 0.43              |
| 52:BT:29:ARG:HH11  | 52:BT:88:ILE:CD1   | 2.24                     | 0.43              |
| 52:BT:34:VAL:HG22  | 52:BT:39:ARG:CA    | 2.48                     | 0.43              |
| 57:BY:28:LYS:HA    | 57:BY:38:ILE:CG2   | 2.34                     | 0.43              |
| 57:BY:28:LYS:HE2   | 57:BY:28:LYS:N     | 2.34                     | 0.43              |
| 58:BZ:74:VAL:CG2   | 58:BZ:86:VAL:HG13  | 2.42                     | 0.43              |
| 1:AA:1460:A:H2'    | 1:AA:1461:G:O4'    | 2.17                     | 0.43              |
| 1:AA:185:A:C5      | 1:AA:186:C:C4      | 3.06                     | 0.43              |
| 1:AA:321:A:H2'     | 1:AA:322:C:H5'     | 1.99                     | 0.43              |
| 1:AA:937:A:H2'     | 1:AA:938:A:H8      | 1.84                     | 0.43              |
| 3:AC:132:ARG:O     | 3:AC:136:GLN:HB2   | 2.18                     | 0.43              |
| 3:AC:180:ALA:O     | 3:AC:181:ASN:CB    | 2.66                     | 0.43              |
| 7:AG:51:GLN:O      | 7:AG:52:GLU:CB     | 2.65                     | 0.43              |
| 19:AS:19:VAL:O     | 19:AS:22:LEU:HB3   | 2.18                     | 0.43              |
| 24:AY:12:LEU:O     | 24:AY:13:ARG:HD2   | 2.19                     | 0.43              |
| 24:AY:153:MET:HA   | 24:AY:157:LEU:CD2  | 2.46                     | 0.43              |
| 24:AY:15:ILE:HA    | 24:AY:103:GLY:O    | 2.18                     | 0.43              |
| 24:AY:229:LEU:HA   | 24:AY:232:LEU:HD22 | 2.00                     | 0.43              |
| 24:AY:348:ARG:NH1  | 24:AY:382:GLU:HG3  | 2.33                     | 0.43              |
| 24:AY:606:MET:CE   | 24:AY:671:MET:HG3  | 2.48                     | 0.43              |
| 24:AY:684:GLN:O    | 24:AY:687:LEU:HB2  | 2.17                     | 0.43              |
| 33:B8:29:LYS:HD3   | 33:B8:44:LYS:HB2   | 1.97                     | 0.43              |
| 35:BA:1122:G:C2    | 35:BA:1123:C:C6    | 3.07                     | 0.43              |
| 35:BA:1137:G:H2'   | 35:BA:1138:G:H8    | 1.81                     | 0.43              |
| 35:BA:1300:U:C1'   | 35:BA:1301:A:OP2   | 2.67                     | 0.43              |
| 35:BA:769:G:H4'    | 35:BA:1379:A:N6    | 2.33                     | 0.43              |
| 35:BA:1424:G:H2'   | 35:BA:1425:G:H8    | 1.82                     | 0.43              |
| 35:BA:1496:A:O3'   | 35:BA:1497:U:O2    | 2.36                     | 0.43              |
| 35:BA:1642:G:H8    | 35:BA:1642:G:O5'   | 2.02                     | 0.43              |
| 35:BA:1710:C:H4'   | 35:BA:2858:C:O2    | 2.18                     | 0.43              |
| 35:BA:1748:G:C8    | 35:BA:1748:G:H5'   | 2.43                     | 0.43              |
| 35:BA:1770:G:H2'   | 35:BA:1771:C:C6    | 2.53                     | 0.43              |
| 35:BA:2137:C:N3    | 35:BA:2154:G:O6    | 2.52                     | 0.43              |
| 35:BA:2298:A:N6    | 35:BA:2318:G:H8    | 2.14                     | 0.43              |
| 35:BA:2607:G:C2'   | 35:BA:2608:G:O5'   | 2.66                     | 0.43              |
| 35:BA:19:C:H5'     | 35:BA:554:U:OP1    | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BB:87:G:C2'     | 36:BB:88:C:H5''    | 2.45                     | 0.43              |
| 37:BC:194:ILE:HD11 | 37:BC:227:PRO:HB2  | 1.99                     | 0.43              |
| 38:BD:72:LYS:HE2   | 38:BD:101:GLU:CD   | 2.38                     | 0.43              |
| 35:BA:2032:G:N2    | 39:BE:146:THR:CG2  | 2.58                     | 0.43              |
| 41:BG:49:ASP:O     | 41:BG:52:ILE:N     | 2.50                     | 0.43              |
| 46:BN:78:TYR:N     | 46:BN:78:TYR:CD1   | 2.87                     | 0.43              |
| 48:BP:38:GLN:CG    | 48:BP:39:LYS:H     | 2.18                     | 0.43              |
| 51:BS:53:SER:C     | 51:BS:55:ALA:H     | 2.22                     | 0.43              |
| 53:BU:64:ARG:O     | 53:BU:65:ILE:C     | 2.56                     | 0.43              |
| 57:BY:59:GLY:C     | 57:BY:60:PHE:HD1   | 2.21                     | 0.43              |
| 57:BY:77:PRO:O     | 57:BY:78:ALA:HB2   | 2.17                     | 0.43              |
| 57:BY:81:LYS:HA    | 57:BY:82:PRO:HD3   | 1.78                     | 0.43              |
| 58:BZ:180:VAL:HG13 | 58:BZ:181:GLU:H    | 1.73                     | 0.43              |
| 1:AA:951:G:C6      | 1:AA:1231:G:C6     | 3.06                     | 0.43              |
| 1:AA:1456:G:H2'    | 1:AA:1456:G:N3     | 2.34                     | 0.43              |
| 1:AA:412:A:H4'     | 1:AA:413:G:H8      | 1.82                     | 0.43              |
| 1:AA:41:G:H2'      | 1:AA:42:G:H8       | 1.84                     | 0.43              |
| 1:AA:488:C:C2'     | 1:AA:489:C:H5'     | 2.48                     | 0.43              |
| 1:AA:51:A:H4'      | 1:AA:52:G:C5'      | 2.49                     | 0.43              |
| 1:AA:774:G:H2'     | 1:AA:775:G:C5'     | 2.48                     | 0.43              |
| 1:AA:779:C:H2'     | 1:AA:780:A:O4'     | 2.18                     | 0.43              |
| 4:AD:150:GLU:C     | 4:AD:152:SER:H     | 2.21                     | 0.43              |
| 8:AH:1:MET:CE      | 8:AH:1:MET:N       | 2.81                     | 0.43              |
| 9:AI:110:GLU:OE2   | 9:AI:113:LYS:NZ    | 2.52                     | 0.43              |
| 9:AI:41:VAL:O      | 9:AI:41:VAL:HG12   | 2.19                     | 0.43              |
| 13:AM:70:LEU:O     | 13:AM:73:GLU:N     | 2.51                     | 0.43              |
| 1:AA:1314:C:OP2    | 19:AS:6:LYS:HD2    | 2.18                     | 0.43              |
| 24:AY:164:MET:C    | 24:AY:180:VAL:HG22 | 2.39                     | 0.43              |
| 24:AY:170:ARG:HD2  | 24:AY:170:ARG:N    | 2.32                     | 0.43              |
| 24:AY:225:GLU:O    | 24:AY:228:MET:HB3  | 2.18                     | 0.43              |
| 24:AY:33:LEU:HD23  | 24:AY:360:ALA:CB   | 2.48                     | 0.43              |
| 24:AY:572:TYR:N    | 24:AY:572:TYR:CD1  | 2.77                     | 0.43              |
| 27:B2:4:SER:C      | 27:B2:6:VAL:N      | 2.72                     | 0.43              |
| 33:B8:33:ASN:N     | 33:B8:36:LYS:HE3   | 2.34                     | 0.43              |
| 34:B9:1:MET:HG3    | 34:B9:1:MET:O      | 2.18                     | 0.43              |
| 35:BA:1142(A):A:C4 | 35:BA:1144:G:C8    | 3.07                     | 0.43              |
| 35:BA:1259:G:O2'   | 35:BA:1260:G:H5'   | 2.18                     | 0.43              |
| 35:BA:1827:C:H2'   | 35:BA:1828:G:C5'   | 2.49                     | 0.43              |
| 35:BA:1970:A:O4'   | 35:BA:1972:A:C8    | 2.72                     | 0.43              |
| 35:BA:1983:C:H4'   | 35:BA:2606:C:O3'   | 2.19                     | 0.43              |
| 35:BA:2036:C:H2'   | 35:BA:2037:G:H5'   | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AV:19:G:O6      | 35:BA:2169:A:H1'   | 2.18                     | 0.43              |
| 35:BA:2175:C:H1'   | 37:BC:218:THR:O    | 2.19                     | 0.43              |
| 35:BA:1669:A:H5''  | 35:BA:2550:G:OP1   | 2.19                     | 0.43              |
| 35:BA:2716:U:C2'   | 35:BA:2717:G:C5'   | 2.84                     | 0.43              |
| 35:BA:448:U:C4     | 35:BA:583:G:H1'    | 2.54                     | 0.43              |
| 35:BA:628:G:O5'    | 35:BA:628:G:H8     | 2.02                     | 0.43              |
| 35:BA:792:G:C3'    | 35:BA:793:A:H5'    | 2.47                     | 0.43              |
| 35:BA:833:U:O4'    | 48:BP:52:GLU:N     | 2.44                     | 0.43              |
| 35:BA:971:C:O2'    | 35:BA:972:G:H5'    | 2.18                     | 0.43              |
| 38:BD:161:THR:O    | 38:BD:162:SER:HB3  | 2.18                     | 0.43              |
| 38:BD:274:ARG:HB3  | 38:BD:275:LYS:H    | 1.73                     | 0.43              |
| 38:BD:45:ASN:CG    | 38:BD:46:GLN:N     | 2.71                     | 0.43              |
| 35:BA:1568:G:H5''  | 38:BD:61:LEU:CD2   | 2.49                     | 0.43              |
| 40:BF:201:VAL:HG13 | 40:BF:202:PHE:N    | 2.33                     | 0.43              |
| 41:BG:116:ASP:CG   | 41:BG:117:PHE:H    | 2.21                     | 0.43              |
| 41:BG:60:LEU:HA    | 41:BG:63:ILE:CG2   | 2.49                     | 0.43              |
| 29:B4:6:HIS:HE1    | 41:BG:66:GLN:HB2   | 1.82                     | 0.43              |
| 48:BP:98:GLU:O     | 48:BP:101:VAL:HG22 | 2.17                     | 0.43              |
| 39:BE:27:LEU:HD23  | 52:BT:1:MET:HB2    | 2.00                     | 0.43              |
| 55:BW:10:VAL:O     | 55:BW:11:ARG:HB2   | 2.19                     | 0.43              |
| 1:AA:223:U:H2'     | 1:AA:224:C:H6      | 1.83                     | 0.43              |
| 1:AA:441:A:H3'     | 1:AA:442:C:H6      | 1.84                     | 0.43              |
| 1:AA:508:C:C4'     | 1:AA:509:A:O5'     | 2.49                     | 0.43              |
| 1:AA:560:U:C5'     | 1:AA:561:U:O5'     | 2.66                     | 0.43              |
| 1:AA:594:G:H2'     | 1:AA:595:G:O5'     | 2.18                     | 0.43              |
| 1:AA:691:G:H2'     | 1:AA:692:U:C6      | 2.53                     | 0.43              |
| 1:AA:911:U:H2'     | 1:AA:912:C:C6      | 2.54                     | 0.43              |
| 1:AA:982:U:HO2'    | 1:AA:983:A:P       | 2.41                     | 0.43              |
| 1:AA:992:U:H4'     | 1:AA:993:G:O5'     | 2.18                     | 0.43              |
| 2:AB:238:LEU:O     | 2:AB:239:VAL:C     | 2.55                     | 0.43              |
| 2:AB:73:THR:O      | 2:AB:74:LYS:C      | 2.57                     | 0.43              |
| 3:AC:118:GLN:O     | 3:AC:119:ARG:C     | 2.57                     | 0.43              |
| 7:AG:36:LYS:O      | 7:AG:38:LEU:N      | 2.51                     | 0.43              |
| 7:AG:41:ARG:O      | 7:AG:42:ILE:C      | 2.57                     | 0.43              |
| 9:AI:118:LYS:O     | 9:AI:119:ALA:CB    | 2.66                     | 0.43              |
| 12:AL:117:ARG:HD2  | 12:AL:122:THR:OG1  | 2.19                     | 0.43              |
| 12:AL:41:ARG:NH1   | 12:AL:43:VAL:HG22  | 2.26                     | 0.43              |
| 14:AN:12:ARG:HB3   | 14:AN:14:PRO:HD2   | 2.00                     | 0.43              |
| 17:AQ:26:GLN:HA    | 17:AQ:36:ILE:O     | 2.18                     | 0.43              |
| 24:AY:102:ASP:O    | 24:AY:130:VAL:HG13 | 2.17                     | 0.43              |
| 24:AY:148:LEU:O    | 24:AY:152:THR:CG2  | 2.66                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:484:ARG:HA   | 24:AY:484:ARG:HD3  | 1.83                     | 0.43              |
| 24:AY:530:VAL:CG2  | 24:AY:531:GLY:N    | 2.74                     | 0.43              |
| 24:AY:615:GLU:HG3  | 24:AY:615:GLU:H    | 1.55                     | 0.43              |
| 24:AY:610:VAL:CG2  | 24:AY:643:ILE:HB   | 2.48                     | 0.43              |
| 28:B3:31:LEU:C     | 28:B3:33:GLN:H     | 2.18                     | 0.43              |
| 35:BA:1036:G:O2'   | 35:BA:1037:G:H5'   | 2.18                     | 0.43              |
| 35:BA:1208:C:C4    | 35:BA:1209:G:N7    | 2.86                     | 0.43              |
| 35:BA:1490:A:C2    | 38:BD:75:ILE:HD13  | 2.54                     | 0.43              |
| 35:BA:1348:G:C2    | 35:BA:1599:C:N3    | 2.87                     | 0.43              |
| 35:BA:1649:G:C2'   | 35:BA:1650:G:C5'   | 2.95                     | 0.43              |
| 35:BA:1652:A:C6    | 35:BA:1653:G:N1    | 2.86                     | 0.43              |
| 25:B0:18:ALA:HB1   | 35:BA:2271:G:OP1   | 2.19                     | 0.43              |
| 35:BA:2310:A:N7    | 41:BG:75:LYS:CE    | 2.82                     | 0.43              |
| 35:BA:2350:C:H2'   | 35:BA:2351:G:O4'   | 2.18                     | 0.43              |
| 35:BA:2753:A:H2'   | 35:BA:2754:U:C6    | 2.53                     | 0.43              |
| 35:BA:500:G:H22    | 35:BA:502:A:H3'    | 1.80                     | 0.43              |
| 35:BA:56:A:H2'     | 35:BA:57:C:O4'     | 2.19                     | 0.43              |
| 35:BA:653:A:C4'    | 35:BA:654:A:OP2    | 2.64                     | 0.43              |
| 37:BC:104:ILE:HD12 | 37:BC:104:ILE:O    | 2.18                     | 0.43              |
| 37:BC:11:LEU:HD11  | 37:BC:35:THR:HG23  | 2.01                     | 0.43              |
| 37:BC:149:ASN:ND2  | 37:BC:152:GLU:HB3  | 2.23                     | 0.43              |
| 37:BC:78:ILE:O     | 37:BC:78:ILE:HG22  | 2.19                     | 0.43              |
| 39:BE:105:THR:OG1  | 39:BE:199:ARG:NH2  | 2.45                     | 0.43              |
| 39:BE:116:VAL:HG13 | 39:BE:122:PHE:CB   | 2.49                     | 0.43              |
| 41:BG:137:GLU:O    | 41:BG:138:GLN:C    | 2.57                     | 0.43              |
| 41:BG:139:LEU:N    | 41:BG:139:LEU:HD23 | 2.34                     | 0.43              |
| 46:BN:109:LYS:HB2  | 46:BN:109:LYS:HE3  | 1.83                     | 0.43              |
| 52:BT:38:ASN:N     | 52:BT:38:ASN:ND2   | 2.63                     | 0.43              |
| 54:BV:38:LEU:HD23  | 54:BV:39:LEU:N     | 2.34                     | 0.43              |
| 54:BV:46:VAL:O     | 54:BV:48:GLY:N     | 2.51                     | 0.43              |
| 57:BY:43:ASN:CG    | 57:BY:43:ASN:O     | 2.57                     | 0.43              |
| 57:BY:79:CYS:O     | 57:BY:80:GLY:O     | 2.35                     | 0.43              |
| 57:BY:81:LYS:HG3   | 57:BY:97:ARG:HD3   | 2.00                     | 0.43              |
| 1:AA:115:G:O4'     | 1:AA:116:A:OP2     | 2.36                     | 0.43              |
| 1:AA:124:G:C6      | 1:AA:125:U:C4      | 3.06                     | 0.43              |
| 1:AA:1502:A:H4'    | 1:AA:1503:A:OP2    | 2.18                     | 0.43              |
| 1:AA:299:G:H2'     | 1:AA:300:A:C8      | 2.53                     | 0.43              |
| 1:AA:964:A:H8      | 1:AA:964:A:O5'     | 2.01                     | 0.43              |
| 3:AC:6:HIS:CB      | 14:AN:49:HIS:HB3   | 2.48                     | 0.43              |
| 14:AN:4:LYS:HA     | 14:AN:7:ILE:HG12   | 1.99                     | 0.43              |
| 18:AR:26:LEU:HD13  | 18:AR:39:VAL:HG13  | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AV:41:C:H2'     | 22:AV:42:C:C5'     | 2.47                     | 0.43              |
| 24:AY:165:GLN:HB2  | 24:AY:260:LEU:HD13 | 1.99                     | 0.43              |
| 27:B2:2:LYS:HD2    | 27:B2:5:GLU:CG     | 2.45                     | 0.43              |
| 28:B3:32:GLN:O     | 28:B3:33:GLN:C     | 2.56                     | 0.43              |
| 35:BA:1092:C:O2'   | 35:BA:1093:G:H5'   | 2.17                     | 0.43              |
| 35:BA:1145:C:H6    | 35:BA:1145:C:O5'   | 2.01                     | 0.43              |
| 35:BA:1171:G:H2'   | 35:BA:1171:G:N3    | 2.34                     | 0.43              |
| 35:BA:1445:A:H8    | 35:BA:1460:A:C5    | 2.36                     | 0.43              |
| 35:BA:1654:A:C1'   | 35:BA:2823:A:H5'   | 2.48                     | 0.43              |
| 35:BA:1782:C:H1'   | 35:BA:2609:U:C5'   | 2.46                     | 0.43              |
| 35:BA:1786:A:H1'   | 35:BA:1938:A:H61   | 1.77                     | 0.43              |
| 35:BA:18:C:C4      | 35:BA:19:C:N4      | 2.87                     | 0.43              |
| 35:BA:2086:U:H2'   | 35:BA:2087:G:C8    | 2.52                     | 0.43              |
| 35:BA:2192:G:HO2'  | 35:BA:2193:G:H5''  | 1.83                     | 0.43              |
| 35:BA:2230:G:C6    | 35:BA:2231:C:C4    | 3.06                     | 0.43              |
| 35:BA:2554:U:C2'   | 35:BA:2555:U:H5'   | 2.49                     | 0.43              |
| 35:BA:270:A:H2'    | 35:BA:271:A:O4'    | 2.19                     | 0.43              |
| 35:BA:2833:G:H3'   | 35:BA:2834:G:C5'   | 2.49                     | 0.43              |
| 37:BC:73:VAL:CG1   | 37:BC:74:ARG:N     | 2.82                     | 0.43              |
| 35:BA:1820:U:H3    | 38:BD:160:GLY:HA3  | 1.84                     | 0.43              |
| 39:BE:154:LYS:O    | 39:BE:154:LYS:HG2  | 2.18                     | 0.43              |
| 39:BE:45:THR:O     | 39:BE:46:ALA:HB2   | 2.18                     | 0.43              |
| 40:BF:203:GLN:C    | 40:BF:205:ARG:N    | 2.72                     | 0.43              |
| 40:BF:83:PHE:O     | 40:BF:84:VAL:C     | 2.57                     | 0.43              |
| 35:BA:2306:C:H4'   | 41:BG:136:ARG:NH1  | 2.34                     | 0.43              |
| 41:BG:172:LEU:CD2  | 41:BG:176:LEU:HD12 | 2.48                     | 0.43              |
| 42:BH:125:VAL:O    | 42:BH:125:VAL:HG12 | 2.17                     | 0.43              |
| 48:BP:125:VAL:HG11 | 48:BP:138:LEU:HD21 | 2.01                     | 0.43              |
| 49:BQ:50:ALA:HB1   | 49:BQ:121:ALA:HB1  | 2.00                     | 0.43              |
| 49:BQ:58:PHE:CD1   | 49:BQ:58:PHE:O     | 2.70                     | 0.43              |
| 51:BS:89:ARG:CB    | 51:BS:92:TYR:HB3   | 2.48                     | 0.43              |
| 52:BT:27:THR:O     | 52:BT:28:VAL:CG1   | 2.66                     | 0.43              |
| 52:BT:6:LEU:C      | 52:BT:8:LYS:N      | 2.72                     | 0.43              |
| 52:BT:62:THR:CG2   | 52:BT:75:ILE:HG12  | 2.46                     | 0.43              |
| 53:BU:85:LYS:C     | 53:BU:87:GLY:H     | 2.22                     | 0.43              |
| 54:BV:21:ARG:HG2   | 54:BV:21:ARG:NH1   | 2.34                     | 0.43              |
| 56:BX:21:PHE:N     | 56:BX:21:PHE:CD1   | 2.87                     | 0.43              |
| 58:BZ:151:HIS:HB2  | 58:BZ:171:ILE:H    | 1.83                     | 0.43              |
| 58:BZ:185:GLU:HG2  | 58:BZ:187:ALA:N    | 2.33                     | 0.43              |
| 1:AA:1145:C:O2'    | 1:AA:1146:A:H8     | 2.01                     | 0.43              |
| 1:AA:1267:C:N4     | 1:AA:1327:C:O2'    | 2.51                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1366:C:N4     | 1:AA:1367:C:N4     | 2.66                     | 0.43              |
| 1:AA:1403:C:H2'    | 1:AA:1404:C:C6     | 2.54                     | 0.43              |
| 1:AA:406:G:C4      | 1:AA:495:A:C6      | 3.06                     | 0.43              |
| 1:AA:453:A:O2'     | 1:AA:454:C:H6      | 1.99                     | 0.43              |
| 1:AA:524:G:O5'     | 1:AA:524:G:H8      | 2.02                     | 0.43              |
| 1:AA:650:G:O2'     | 1:AA:651:C:H5'     | 2.19                     | 0.43              |
| 2:AB:58:ILE:HG22   | 2:AB:222:ILE:HD13  | 2.01                     | 0.43              |
| 4:AD:106:TYR:C     | 4:AD:108:LEU:H     | 2.22                     | 0.43              |
| 5:AE:20:GLN:HE21   | 5:AE:20:GLN:HB3    | 1.54                     | 0.43              |
| 7:AG:122:HIS:HD2   | 7:AG:125:MET:CE    | 2.31                     | 0.43              |
| 9:AI:97:LYS:HB3    | 9:AI:98:PRO:HD3    | 2.01                     | 0.43              |
| 14:AN:4:LYS:O      | 14:AN:7:ILE:HG12   | 2.19                     | 0.43              |
| 15:AO:23:GLY:O     | 15:AO:27:VAL:HB    | 2.19                     | 0.43              |
| 19:AS:66:MET:HE3   | 19:AS:74:PHE:CE2   | 2.54                     | 0.43              |
| 20:AT:71:THR:HG22  | 20:AT:72:LEU:H     | 1.84                     | 0.43              |
| 24:AY:199:ILE:C    | 24:AY:199:ILE:HD12 | 2.39                     | 0.43              |
| 24:AY:403:GLU:O    | 24:AY:404:VAL:HB   | 2.19                     | 0.43              |
| 24:AY:464:ASP:O    | 24:AY:468:ARG:HG3  | 2.19                     | 0.43              |
| 24:AY:58:GLU:O     | 24:AY:60:GLU:N     | 2.51                     | 0.43              |
| 25:B0:45:PHE:O     | 25:B0:59:LEU:HD11  | 2.19                     | 0.43              |
| 25:B0:49:LYS:N     | 25:B0:80:HIS:HB3   | 2.33                     | 0.43              |
| 28:B3:47:VAL:CG1   | 28:B3:56:VAL:HG21  | 2.48                     | 0.43              |
| 31:B6:9:LEU:HD22   | 31:B6:10:LEU:N     | 2.33                     | 0.43              |
| 34:B9:9:ARG:O      | 34:B9:10:ILE:O     | 2.36                     | 0.43              |
| 35:BA:1079:C:O2    | 35:BA:1079:C:C2'   | 2.58                     | 0.43              |
| 35:BA:1115:G:H2'   | 35:BA:1116:C:O4'   | 2.19                     | 0.43              |
| 35:BA:1227:G:C2    | 35:BA:1228:G:C8    | 3.07                     | 0.43              |
| 35:BA:171:G:C2'    | 35:BA:172:C:H5'    | 2.48                     | 0.43              |
| 35:BA:2033:A:H8    | 35:BA:2033:A:O5'   | 2.01                     | 0.43              |
| 35:BA:2029:G:N1    | 35:BA:2033:A:OP2   | 2.32                     | 0.43              |
| 35:BA:2103:C:H4'   | 35:BA:2104:G:OP1   | 2.19                     | 0.43              |
| 35:BA:1890:A:H2    | 35:BA:2235:G:O4'   | 2.02                     | 0.43              |
| 35:BA:2318:G:H2'   | 35:BA:2319:G:OP1   | 2.19                     | 0.43              |
| 35:BA:2600:A:O2'   | 35:BA:2601:C:H5'   | 2.19                     | 0.43              |
| 35:BA:890:A:H2'    | 35:BA:892:G:C5'    | 2.48                     | 0.43              |
| 37:BC:195:ARG:HH11 | 37:BC:195:ARG:HG3  | 1.83                     | 0.43              |
| 37:BC:89:GLU:OE2   | 37:BC:90:ALA:HB2   | 2.19                     | 0.43              |
| 39:BE:128:SER:O    | 39:BE:129:HIS:HB2  | 2.19                     | 0.43              |
| 39:BE:202:LYS:HD2  | 39:BE:202:LYS:N    | 2.33                     | 0.43              |
| 39:BE:70:ALA:O     | 39:BE:72:VAL:N     | 2.52                     | 0.43              |
| 40:BF:149:ASP:OD1  | 40:BF:149:ASP:N    | 2.50                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:87:PRO:O     | 41:BG:88:ILE:CB    | 2.67                     | 0.43              |
| 42:BH:87:LEU:N     | 42:BH:131:VAL:O    | 2.40                     | 0.43              |
| 44:BK:105:UNK:O    | 44:BK:106:UNK:C    | 2.65                     | 0.43              |
| 44:BK:128:UNK:C    | 44:BK:130:UNK:N    | 2.81                     | 0.43              |
| 50:BR:100:LEU:HD22 | 50:BR:112:ALA:HA   | 2.00                     | 0.43              |
| 35:BA:2839:G:H5'   | 50:BR:46:GLY:HA2   | 2.01                     | 0.43              |
| 50:BR:59:ASP:O     | 50:BR:60:LEU:CB    | 2.65                     | 0.43              |
| 52:BT:89:VAL:CB    | 52:BT:91:ARG:HG3   | 2.43                     | 0.43              |
| 53:BU:76:TYR:CE1   | 53:BU:80:ILE:HG13  | 2.54                     | 0.43              |
| 53:BU:83:LEU:CG    | 53:BU:88:ILE:HD11  | 2.48                     | 0.43              |
| 54:BV:5:VAL:HG23   | 54:BV:37:VAL:HG23  | 2.01                     | 0.43              |
| 56:BX:11:PRO:HB3   | 56:BX:92:LEU:CD2   | 2.48                     | 0.43              |
| 57:BY:29:GLU:N     | 57:BY:29:GLU:CD    | 2.71                     | 0.43              |
| 35:BA:329:G:P      | 57:BY:71:LYS:HD3   | 2.59                     | 0.43              |
| 1:AA:116:A:H8      | 1:AA:116:A:O5'     | 2.02                     | 0.43              |
| 1:AA:1327:C:OP2    | 21:AU:12:LYS:NZ    | 2.52                     | 0.43              |
| 1:AA:160:A:H1'     | 1:AA:344:A:C6      | 2.54                     | 0.43              |
| 1:AA:198:G:N3      | 1:AA:199:G:C5      | 2.87                     | 0.43              |
| 1:AA:266:G:HO2'    | 1:AA:267:C:P       | 2.39                     | 0.43              |
| 1:AA:376:G:H5''    | 16:AP:5:ARG:HD2    | 2.01                     | 0.43              |
| 1:AA:474:G:O2'     | 1:AA:475:G:H5'     | 2.18                     | 0.43              |
| 1:AA:523:A:C2      | 12:AL:91:LYS:HB3   | 2.53                     | 0.43              |
| 3:AC:84:ILE:O      | 3:AC:85:ARG:C      | 2.57                     | 0.43              |
| 7:AG:127:ALA:O     | 7:AG:129:GLU:N     | 2.52                     | 0.43              |
| 7:AG:49:ILE:HD11   | 7:AG:117:ALA:O     | 2.19                     | 0.43              |
| 9:AI:48:GLU:CD     | 9:AI:51:ARG:HD3    | 2.39                     | 0.43              |
| 15:AO:68:ARG:CG    | 15:AO:68:ARG:HH11  | 2.31                     | 0.43              |
| 19:AS:41:VAL:CG2   | 19:AS:44:MET:HG3   | 2.49                     | 0.43              |
| 20:AT:72:LEU:HD21  | 20:AT:80:ARG:HE    | 1.83                     | 0.43              |
| 22:AV:27:G:N2      | 22:AV:43:C:H5      | 2.07                     | 0.43              |
| 24:AY:213:HIS:O    | 24:AY:217:VAL:HG23 | 2.19                     | 0.43              |
| 26:B1:58:ILE:HD11  | 26:B1:90:ILE:HG21  | 2.00                     | 0.43              |
| 30:B5:41:PRO:HA    | 30:B5:42:PRO:HD3   | 1.80                     | 0.43              |
| 35:BA:1054:A:C2    | 35:BA:1106:G:C6    | 3.07                     | 0.43              |
| 35:BA:1858:G:H8    | 35:BA:1858:G:OP2   | 2.02                     | 0.43              |
| 35:BA:1902:C:H4'   | 38:BD:244:ARG:CB   | 2.49                     | 0.43              |
| 35:BA:2012:G:H4'   | 55:BW:96:ILE:CD1   | 2.49                     | 0.43              |
| 35:BA:2313:C:H2'   | 35:BA:2314:C:C6    | 2.54                     | 0.43              |
| 35:BA:2423:U:C6    | 35:BA:2423:U:H5'   | 2.49                     | 0.43              |
| 35:BA:2482:G:C2    | 35:BA:2483:C:H1'   | 2.53                     | 0.43              |
| 35:BA:2579:C:H2'   | 35:BA:2580:U:O4'   | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2758:A:C2    | 35:BA:2759:G:H1'   | 2.53                     | 0.43              |
| 35:BA:341:G:O2'    | 35:BA:342:G:H5'    | 2.18                     | 0.43              |
| 35:BA:385:C:O2     | 48:BP:71:VAL:HG21  | 2.19                     | 0.43              |
| 35:BA:634:C:H2'    | 35:BA:635:C:C6     | 2.53                     | 0.43              |
| 35:BA:652:C:O2'    | 35:BA:653:A:C4     | 2.71                     | 0.43              |
| 35:BA:814:C:H2'    | 35:BA:815:C:H6     | 1.82                     | 0.43              |
| 35:BA:847:U:H2'    | 35:BA:848:G:H5''   | 1.99                     | 0.43              |
| 35:BA:848:G:H5'    | 35:BA:848:G:C8     | 2.49                     | 0.43              |
| 37:BC:103:LYS:O    | 37:BC:104:ILE:C    | 2.57                     | 0.43              |
| 37:BC:138:LEU:HA   | 37:BC:139:PRO:HD2  | 1.91                     | 0.43              |
| 37:BC:225:ILE:O    | 37:BC:227:PRO:HD3  | 2.19                     | 0.43              |
| 37:BC:90:ALA:HB1   | 37:BC:155:ARG:HG2  | 2.01                     | 0.43              |
| 38:BD:31:LYS:NZ    | 38:BD:102:LYS:NZ   | 2.67                     | 0.43              |
| 35:BA:2580:U:O3'   | 39:BE:130:GLY:HA2  | 2.19                     | 0.43              |
| 40:BF:157:VAL:O    | 40:BF:194:MET:HA   | 2.18                     | 0.43              |
| 40:BF:167:ALA:HA   | 40:BF:170:LEU:HD23 | 2.01                     | 0.43              |
| 41:BG:104:GLU:H    | 41:BG:107:LEU:H    | 1.67                     | 0.43              |
| 41:BG:182:LYS:OXT  | 41:BG:182:LYS:CD   | 2.66                     | 0.43              |
| 46:BN:1:MET:SD     | 46:BN:2:LYS:C      | 2.97                     | 0.43              |
| 47:BO:8:LEU:HD13   | 47:BO:82:ASN:HB3   | 2.00                     | 0.43              |
| 48:BP:146:VAL:HG13 | 48:BP:147:LEU:H    | 1.81                     | 0.43              |
| 49:BQ:54:MET:HB3   | 49:BQ:64:ILE:HD11  | 1.99                     | 0.43              |
| 52:BT:58:ASN:ND2   | 52:BT:58:ASN:N     | 2.58                     | 0.43              |
| 54:BV:2:PHE:CD1    | 54:BV:3:ALA:N      | 2.87                     | 0.43              |
| 56:BX:12:VAL:HG12  | 56:BX:29:TRP:CE2   | 2.53                     | 0.43              |
| 57:BY:31:LEU:HB2   | 57:BY:32:PRO:HA    | 2.01                     | 0.43              |
| 57:BY:7:VAL:HB     | 57:BY:8:LYS:HZ1    | 1.76                     | 0.43              |
| 1:AA:1081:G:O6     | 5:AE:47:LYS:NZ     | 2.41                     | 0.43              |
| 1:AA:1184:G:H2'    | 1:AA:1185:G:H5'    | 1.98                     | 0.43              |
| 1:AA:1217:C:O2'    | 1:AA:1218:C:H5'    | 2.19                     | 0.43              |
| 1:AA:1238:A:C8     | 1:AA:1303:C:H1'    | 2.54                     | 0.43              |
| 1:AA:382:A:H2'     | 1:AA:383:A:C8      | 2.54                     | 0.43              |
| 1:AA:563:A:N3      | 1:AA:563:A:H2'     | 2.34                     | 0.43              |
| 1:AA:865:A:H2'     | 1:AA:866:C:C6      | 2.54                     | 0.43              |
| 2:AB:231:GLU:CB    | 2:AB:232:PRO:HD3   | 2.33                     | 0.43              |
| 4:AD:104:VAL:HG11  | 4:AD:146:ILE:HG13  | 2.01                     | 0.43              |
| 4:AD:38:TYR:N      | 4:AD:38:TYR:CD1    | 2.87                     | 0.43              |
| 7:AG:19:GLY:O      | 7:AG:20:ASP:CB     | 2.66                     | 0.43              |
| 9:AI:52:ALA:HB3    | 9:AI:95:LYS:HZ3    | 1.82                     | 0.43              |
| 19:AS:22:LEU:HD11  | 19:AS:27:GLU:H     | 1.84                     | 0.43              |
| 1:AA:192:U:H1'     | 20:AT:103:GLY:CA   | 2.49                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:153:MET:O    | 24:AY:157:LEU:HD23 | 2.18                     | 0.43              |
| 24:AY:251:ILE:HD13 | 24:AY:285:ASP:HB3  | 2.00                     | 0.43              |
| 24:AY:517:LEU:CD1  | 24:AY:517:LEU:N    | 2.80                     | 0.43              |
| 24:AY:658:ASP:O    | 24:AY:662:LYS:HG2  | 2.19                     | 0.43              |
| 24:AY:681:LYS:O    | 24:AY:684:GLN:HB3  | 2.19                     | 0.43              |
| 24:AY:82:ILE:O     | 24:AY:83:ASP:C     | 2.57                     | 0.43              |
| 24:AY:9:LEU:HD22   | 24:AY:284:LEU:HD22 | 2.00                     | 0.43              |
| 27:B2:69:ARG:C     | 27:B2:70:GLN:CD    | 2.78                     | 0.43              |
| 27:B2:70:GLN:O     | 27:B2:71:ASN:O     | 2.36                     | 0.43              |
| 28:B3:2:PRO:HG2    | 28:B3:39:ASP:HB3   | 2.01                     | 0.43              |
| 29:B4:50:VAL:O     | 29:B4:51:ASP:C     | 2.57                     | 0.43              |
| 31:B6:12:GLU:OE1   | 31:B6:52:VAL:HG13  | 2.19                     | 0.43              |
| 33:B8:32:LEU:O     | 33:B8:33:ASN:O     | 2.36                     | 0.43              |
| 35:BA:108:U:H2'    | 35:BA:109:G:H5'    | 1.98                     | 0.43              |
| 35:BA:1283:G:H2'   | 35:BA:1285:G:OP2   | 2.19                     | 0.43              |
| 35:BA:1332:G:H4'   | 35:BA:1333:C:OP2   | 2.18                     | 0.43              |
| 35:BA:154:G:O2'    | 35:BA:154(A):C:H5' | 2.18                     | 0.43              |
| 35:BA:1478:G:O2'   | 35:BA:1558:A:C2    | 2.72                     | 0.43              |
| 35:BA:1794:U:H2'   | 35:BA:1795:C:C6    | 2.54                     | 0.43              |
| 35:BA:16:G:HO2'    | 35:BA:17:G:H5'     | 1.79                     | 0.43              |
| 35:BA:1801:G:C6    | 35:BA:2202:C:O4'   | 2.71                     | 0.43              |
| 32:B7:32:LYS:HE2   | 35:BA:180:G:OP2    | 2.19                     | 0.43              |
| 35:BA:2104:G:N7    | 35:BA:2186:G:N2    | 2.67                     | 0.43              |
| 35:BA:301:G:OP2    | 57:BY:97:ARG:NH1   | 2.52                     | 0.43              |
| 35:BA:422:A:H2'    | 35:BA:423:A:C8     | 2.54                     | 0.43              |
| 35:BA:462:C:O2'    | 35:BA:463:G:C5'    | 2.49                     | 0.43              |
| 35:BA:522:G:C6     | 35:BA:523:C:N4     | 2.86                     | 0.43              |
| 35:BA:71:A:H5'     | 35:BA:71:A:C8      | 2.54                     | 0.43              |
| 35:BA:71:A:OP2     | 35:BA:71:A:H3'     | 2.18                     | 0.43              |
| 35:BA:859:G:O3'    | 35:BA:860:U:O2     | 2.37                     | 0.43              |
| 35:BA:92:A:H2'     | 35:BA:93:G:O4'     | 2.19                     | 0.43              |
| 36:BB:28:C:H2'     | 36:BB:29:A:H8      | 1.82                     | 0.43              |
| 37:BC:60:ARG:HG3   | 37:BC:165:ARG:HB2  | 2.01                     | 0.43              |
| 37:BC:195:ARG:HG3  | 37:BC:195:ARG:NH1  | 2.34                     | 0.43              |
| 37:BC:24:ASP:C     | 37:BC:24:ASP:OD1   | 2.55                     | 0.43              |
| 39:BE:24:THR:HB    | 39:BE:184:VAL:HG23 | 2.01                     | 0.43              |
| 39:BE:4:ILE:HG12   | 39:BE:5:LEU:N      | 2.34                     | 0.43              |
| 39:BE:8:LYS:HE2    | 39:BE:192:ASN:HD22 | 1.84                     | 0.43              |
| 40:BF:178:PRO:HB3  | 40:BF:198:ALA:CB   | 2.49                     | 0.43              |
| 41:BG:107:LEU:HD23 | 41:BG:111:LEU:CD1  | 2.49                     | 0.43              |
| 35:BA:2305:A:O2'   | 41:BG:136:ARG:HD2  | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:39:ILE:HD12  | 41:BG:157:ILE:CG1  | 2.39                     | 0.43              |
| 42:BH:86:GLU:CB    | 42:BH:132:ARG:HB3  | 2.48                     | 0.43              |
| 45:BL:85:UNK:O     | 45:BL:86:UNK:C     | 2.67                     | 0.43              |
| 46:BN:36:GLY:HA2   | 46:BN:38:HIS:CE1   | 2.54                     | 0.43              |
| 46:BN:55:VAL:HG22  | 46:BN:56:ASN:H     | 1.83                     | 0.43              |
| 49:BQ:81:VAL:CG1   | 49:BQ:82:ARG:N     | 2.81                     | 0.43              |
| 35:BA:2870:C:H5''  | 50:BR:65:LEU:HD21  | 2.01                     | 0.43              |
| 52:BT:95:ARG:HG2   | 52:BT:95:ARG:H     | 1.67                     | 0.43              |
| 57:BY:28:LYS:O     | 57:BY:38:ILE:N     | 2.52                     | 0.43              |
| 57:BY:50:ARG:C     | 57:BY:52:SER:N     | 2.69                     | 0.43              |
| 58:BZ:144:LEU:HD11 | 58:BZ:150:LEU:H    | 1.84                     | 0.43              |
| 1:AA:262:A:C6      | 1:AA:263:A:C6      | 3.06                     | 0.42              |
| 1:AA:264:U:O2'     | 17:AQ:64:PRO:O     | 2.37                     | 0.42              |
| 1:AA:276:G:O2'     | 1:AA:277:C:H5'     | 2.18                     | 0.42              |
| 1:AA:309:G:C2      | 1:AA:310:G:N7      | 2.87                     | 0.42              |
| 1:AA:519:C:C4      | 1:AA:520:A:C5      | 3.07                     | 0.42              |
| 1:AA:57:G:O2'      | 1:AA:58:C:C5'      | 2.61                     | 0.42              |
| 1:AA:902:G:H2'     | 1:AA:903:G:H8      | 1.84                     | 0.42              |
| 1:AA:960:U:C4      | 1:AA:1225:A:C8     | 3.07                     | 0.42              |
| 2:AB:166:ASP:HB3   | 2:AB:169:LYS:CB    | 2.49                     | 0.42              |
| 2:AB:54:THR:O      | 2:AB:58:ILE:HG13   | 2.19                     | 0.42              |
| 2:AB:97:TRP:HH2    | 2:AB:176:GLU:CD    | 2.22                     | 0.42              |
| 3:AC:103:VAL:HG12  | 3:AC:104:GLN:H     | 1.82                     | 0.42              |
| 3:AC:124:ILE:HG23  | 3:AC:125:GLU:N     | 2.33                     | 0.42              |
| 1:AA:1255:G:OP1    | 3:AC:26:LYS:HE2    | 2.18                     | 0.42              |
| 6:AF:21:LEU:C      | 6:AF:21:LEU:HD13   | 2.40                     | 0.42              |
| 9:AI:10:ARG:HG2    | 9:AI:75:ASP:HB2    | 2.00                     | 0.42              |
| 12:AL:55:VAL:HG22  | 12:AL:56:ALA:H     | 1.83                     | 0.42              |
| 12:AL:83:VAL:CG1   | 12:AL:84:LEU:N     | 2.81                     | 0.42              |
| 13:AM:8:GLU:OE1    | 13:AM:22:ILE:HG12  | 2.19                     | 0.42              |
| 16:AP:11:SER:OG    | 16:AP:12:LYS:N     | 2.51                     | 0.42              |
| 17:AQ:95:TYR:C     | 17:AQ:97:SER:N     | 2.72                     | 0.42              |
| 24:AY:166:LEU:HD13 | 24:AY:180:VAL:HG11 | 2.01                     | 0.42              |
| 24:AY:24:GLY:O     | 24:AY:25:LYS:C     | 2.56                     | 0.42              |
| 24:AY:491:VAL:CG1  | 24:AY:492:ASP:N    | 2.81                     | 0.42              |
| 24:AY:67:ALA:CB    | 24:AY:83:ASP:O     | 2.67                     | 0.42              |
| 29:B4:61:ARG:NH1   | 29:B4:61:ARG:HB2   | 2.32                     | 0.42              |
| 35:BA:1326:U:O2'   | 35:BA:1327:C:H5'   | 2.19                     | 0.42              |
| 35:BA:1446:C:O2    | 35:BA:1446:C:H5''  | 2.19                     | 0.42              |
| 35:BA:1543:C:C3'   | 35:BA:1544:A:C5'   | 2.97                     | 0.42              |
| 35:BA:1643:G:C2'   | 35:BA:1644:C:O5'   | 2.67                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1658:C:H2'   | 35:BA:1659:U:C6    | 2.54                     | 0.42              |
| 35:BA:2007:C:H6    | 35:BA:2007:C:O5'   | 2.02                     | 0.42              |
| 35:BA:2341:G:H2'   | 35:BA:2342:C:C6    | 2.54                     | 0.42              |
| 35:BA:2703:C:H2'   | 35:BA:2704:C:H6    | 1.84                     | 0.42              |
| 35:BA:405:U:H3'    | 35:BA:406:G:H5'    | 2.01                     | 0.42              |
| 35:BA:852:G:H2'    | 35:BA:853:G:H8     | 1.84                     | 0.42              |
| 35:BA:1568:G:H5''  | 38:BD:61:LEU:HD23  | 2.00                     | 0.42              |
| 40:BF:187:VAL:HG12 | 48:BP:7:ARG:HA     | 2.01                     | 0.42              |
| 40:BF:20:LEU:N     | 40:BF:24:LEU:HD23  | 2.30                     | 0.42              |
| 41:BG:51:ARG:O     | 41:BG:52:ILE:HG13  | 2.18                     | 0.42              |
| 42:BH:12:PRO:CD    | 42:BH:76:VAL:HG13  | 2.48                     | 0.42              |
| 42:BH:97:ARG:O     | 42:BH:97:ARG:HG2   | 2.18                     | 0.42              |
| 46:BN:25:ARG:NH1   | 46:BN:25:ARG:CG    | 2.82                     | 0.42              |
| 48:BP:108:LYS:C    | 48:BP:110:TYR:N    | 2.72                     | 0.42              |
| 48:BP:25:SER:O     | 48:BP:30:THR:OG1   | 2.33                     | 0.42              |
| 49:BQ:59:ARG:O     | 49:BQ:59:ARG:HD2   | 2.19                     | 0.42              |
| 35:BA:2334:G:N3    | 51:BS:18:ILE:CD1   | 2.82                     | 0.42              |
| 51:BS:30:ARG:HH11  | 51:BS:97:ARG:CB    | 2.32                     | 0.42              |
| 51:BS:56:LEU:HD23  | 51:BS:56:LEU:O     | 2.19                     | 0.42              |
| 51:BS:62:LYS:C     | 51:BS:64:GLU:H     | 2.22                     | 0.42              |
| 51:BS:39:ILE:CD1   | 51:BS:73:LEU:HD21  | 2.48                     | 0.42              |
| 52:BT:106:SER:HB2  | 52:BT:110:ILE:HG13 | 2.01                     | 0.42              |
| 57:BY:2:ARG:N      | 57:BY:4:LYS:HG2    | 2.34                     | 0.42              |
| 58:BZ:48:PHE:HA    | 58:BZ:51:ALA:HB3   | 2.00                     | 0.42              |
| 1:AA:1425:U:H2'    | 1:AA:1426:C:C6     | 2.54                     | 0.42              |
| 1:AA:1452:C:H4'    | 1:AA:1456:G:O5'    | 2.19                     | 0.42              |
| 1:AA:185:A:N6      | 1:AA:186:C:N4      | 2.67                     | 0.42              |
| 1:AA:751:U:H2'     | 1:AA:752:G:O4'     | 2.19                     | 0.42              |
| 1:AA:942:G:C6      | 1:AA:943:U:O4      | 2.72                     | 0.42              |
| 3:AC:138:VAL:HG21  | 3:AC:168:ALA:HB2   | 1.93                     | 0.42              |
| 5:AE:131:ILE:HD13  | 5:AE:131:ILE:HA    | 1.93                     | 0.42              |
| 1:AA:825:G:N2      | 8:AH:11:THR:HG21   | 2.34                     | 0.42              |
| 9:AI:108:VAL:HG12  | 9:AI:109:VAL:N     | 2.34                     | 0.42              |
| 10:AJ:28:ARG:O     | 10:AJ:30:SER:N     | 2.43                     | 0.42              |
| 10:AJ:90:LEU:N     | 10:AJ:91:PRO:HD3   | 2.29                     | 0.42              |
| 11:AK:14:VAL:HG23  | 11:AK:14:VAL:O     | 2.19                     | 0.42              |
| 11:AK:48:ILE:HG22  | 11:AK:49:GLY:N     | 2.34                     | 0.42              |
| 12:AL:17:LYS:HD3   | 12:AL:18:VAL:N     | 2.26                     | 0.42              |
| 1:AA:520:A:OP2     | 12:AL:51:ALA:HB1   | 2.17                     | 0.42              |
| 12:AL:54:LYS:HD2   | 12:AL:54:LYS:N     | 2.34                     | 0.42              |
| 13:AM:9:ILE:HA     | 13:AM:10:PRO:HD2   | 1.87                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:AM:70:LEU:C     | 13:AM:70:LEU:HD23 | 2.40                     | 0.42              |
| 13:AM:91:ARG:CD    | 13:AM:97:PRO:O    | 2.67                     | 0.42              |
| 20:AT:10:LEU:CD1   | 20:AT:11:SER:H    | 2.26                     | 0.42              |
| 24:AY:96:ARG:NH1   | 24:AY:315:LYS:HG2 | 2.34                     | 0.42              |
| 24:AY:535:PRO:C    | 24:AY:537:GLU:N   | 2.69                     | 0.42              |
| 24:AY:546:ILE:HG22 | 24:AY:547:GLU:N   | 2.34                     | 0.42              |
| 28:B3:6:VAL:HG12   | 28:B3:56:VAL:CG2  | 2.30                     | 0.42              |
| 29:B4:36:CYS:C     | 29:B4:38:LYS:N    | 2.72                     | 0.42              |
| 35:BA:1690:A:H2'   | 35:BA:1691:C:O4'  | 2.19                     | 0.42              |
| 35:BA:1848:A:O2'   | 35:BA:1849:G:H5'  | 2.18                     | 0.42              |
| 35:BA:1937:A:O2'   | 35:BA:1938:A:O5'  | 2.33                     | 0.42              |
| 35:BA:1970:A:O4'   | 35:BA:1972:A:C1'  | 2.67                     | 0.42              |
| 35:BA:1994:C:HO2'  | 35:BA:1995:U:H5'  | 1.79                     | 0.42              |
| 35:BA:2010:G:H2'   | 35:BA:2011:U:H6   | 1.84                     | 0.42              |
| 35:BA:2069:G:C2'   | 35:BA:2070:G:H5'  | 2.49                     | 0.42              |
| 35:BA:2031:A:C6    | 35:BA:2498:C:H1'  | 2.54                     | 0.42              |
| 35:BA:2777:G:C5'   | 35:BA:2778:A:H5'  | 2.47                     | 0.42              |
| 35:BA:49:A:H5''    | 35:BA:51:G:C5'    | 2.49                     | 0.42              |
| 35:BA:548:A:H2'    | 35:BA:549:G:H5'   | 2.01                     | 0.42              |
| 35:BA:792:G:H3'    | 35:BA:793:A:H5'   | 2.01                     | 0.42              |
| 37:BC:54:ARG:HE    | 37:BC:57:GLN:HG2  | 1.83                     | 0.42              |
| 35:BA:2635:C:OP1   | 39:BE:77:ILE:HG21 | 2.19                     | 0.42              |
| 40:BF:68:LYS:HB3   | 40:BF:68:LYS:HE3  | 1.69                     | 0.42              |
| 43:BJ:73:UNK:C     | 43:BJ:75:UNK:N    | 2.79                     | 0.42              |
| 44:BK:115:UNK:O    | 44:BK:116:UNK:C   | 2.67                     | 0.42              |
| 46:BN:72:TYR:CD2   | 46:BN:90:MET:HG3  | 2.54                     | 0.42              |
| 47:BO:50:GLY:H     | 47:BO:53:LYS:NZ   | 2.16                     | 0.42              |
| 49:BQ:84:GLY:O     | 49:BQ:85:LYS:HB2  | 2.19                     | 0.42              |
| 51:BS:89:ARG:HG3   | 51:BS:92:TYR:HA   | 2.00                     | 0.42              |
| 52:BT:30:VAL:C     | 52:BT:43:GLN:O    | 2.57                     | 0.42              |
| 53:BU:66:ASN:CG    | 53:BU:76:TYR:HB2  | 2.40                     | 0.42              |
| 53:BU:97:ASP:OD2   | 53:BU:101:ARG:NH1 | 2.52                     | 0.42              |
| 35:BA:309:G:O3'    | 57:BY:18:GLY:HA2  | 2.19                     | 0.42              |
| 57:BY:23:ARG:HH11  | 57:BY:23:ARG:CG   | 2.31                     | 0.42              |
| 58:BZ:53:ILE:HG13  | 58:BZ:54:HIS:HD2  | 1.84                     | 0.42              |
| 1:AA:559:A:N3      | 1:AA:559:A:H2'    | 2.35                     | 0.42              |
| 1:AA:686:U:O4'     | 11:AK:42:TRP:NE1  | 2.39                     | 0.42              |
| 1:AA:803:G:H2'     | 1:AA:804:U:C6     | 2.54                     | 0.42              |
| 2:AB:145:LEU:O     | 2:AB:149:LEU:N    | 2.52                     | 0.42              |
| 2:AB:204:ASN:HD22  | 2:AB:204:ASN:C    | 2.16                     | 0.42              |
| 2:AB:58:ILE:CG2    | 2:AB:222:ILE:HD11 | 2.49                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:AC:38:ARG:NH1     | 3:AC:38:ARG:CB     | 2.82                     | 0.42              |
| 6:AF:15:ASP:C       | 6:AF:17:SER:H      | 2.22                     | 0.42              |
| 6:AF:15:ASP:O       | 6:AF:17:SER:N      | 2.52                     | 0.42              |
| 7:AG:47:CYS:C       | 7:AG:49:ILE:N      | 2.71                     | 0.42              |
| 9:AI:111:ARG:HG2    | 9:AI:112:LYS:N     | 2.33                     | 0.42              |
| 10:AJ:6:ILE:CD1     | 10:AJ:23:ILE:HG21  | 2.48                     | 0.42              |
| 10:AJ:27:ALA:HB2    | 10:AJ:85:LEU:HD11  | 2.01                     | 0.42              |
| 11:AK:67:ASP:OD2    | 11:AK:71:LYS:HE3   | 2.19                     | 0.42              |
| 24:AY:99:ARG:NH2    | 24:AY:128:TYR:CZ   | 2.83                     | 0.42              |
| 24:AY:15:ILE:HD13   | 24:AY:105:ILE:HD13 | 2.01                     | 0.42              |
| 24:AY:166:LEU:HD21  | 24:AY:208:GLN:HG2  | 2.00                     | 0.42              |
| 25:B0:50:ASN:C      | 25:B0:62:LEU:HD21  | 2.39                     | 0.42              |
| 27:B2:69:ARG:NH2    | 35:BA:111:A:H4'    | 2.35                     | 0.42              |
| 28:B3:9:VAL:HG13    | 28:B3:55:ARG:CD    | 2.45                     | 0.42              |
| 31:B6:30:THR:O      | 31:B6:32:ASN:HB2   | 2.19                     | 0.42              |
| 33:B8:12:LYS:HE2    | 48:BP:68:GLN:HG2   | 2.02                     | 0.42              |
| 35:BA:1035:U:H3     | 35:BA:1120:G:H1    | 1.67                     | 0.42              |
| 35:BA:1098:A:C2'    | 35:BA:1099:G:H5'   | 2.49                     | 0.42              |
| 35:BA:1591:G:C8     | 35:BA:1591:G:H5'   | 2.54                     | 0.42              |
| 35:BA:49:A:N7       | 35:BA:177:G:C6     | 2.86                     | 0.42              |
| 35:BA:2199:A:H3'    | 35:BA:2200:C:H6    | 1.84                     | 0.42              |
| 35:BA:479:A:N3      | 35:BA:481:G:H5''   | 2.34                     | 0.42              |
| 35:BA:654(O):G:HO2' | 35:BA:654(P):C:C1' | 2.32                     | 0.42              |
| 35:BA:814:C:H2'     | 35:BA:815:C:C6     | 2.54                     | 0.42              |
| 35:BA:994:C:OP1     | 53:BU:53:ARG:NH2   | 2.52                     | 0.42              |
| 37:BC:153:ILE:O     | 37:BC:157:ILE:HG13 | 2.19                     | 0.42              |
| 35:BA:2174:C:O2     | 37:BC:219:MET:HE3  | 2.19                     | 0.42              |
| 37:BC:97:GLY:O      | 37:BC:100:ILE:HG13 | 2.19                     | 0.42              |
| 38:BD:130:ALA:HA    | 38:BD:192:THR:HA   | 2.00                     | 0.42              |
| 38:BD:33:LEU:HD22   | 38:BD:34:VAL:HG13  | 2.01                     | 0.42              |
| 40:BF:101:LEU:CD1   | 40:BF:102:PRO:HD2  | 2.47                     | 0.42              |
| 40:BF:206:ILE:HG22  | 40:BF:207:GLY:N    | 2.34                     | 0.42              |
| 41:BG:139:LEU:CD2   | 41:BG:139:LEU:N    | 2.81                     | 0.42              |
| 35:BA:2751:G:O6     | 42:BH:1:MET:HG2    | 2.18                     | 0.42              |
| 42:BH:9:ILE:HD12    | 42:BH:69:ARG:HH11  | 1.85                     | 0.42              |
| 44:BK:95:UNK:CB     | 44:BK:135:UNK:HA   | 2.49                     | 0.42              |
| 47:BO:119:PRO:O     | 47:BO:120:GLU:HB2  | 2.19                     | 0.42              |
| 47:BO:63:VAL:HG12   | 47:BO:106:LEU:HD11 | 2.00                     | 0.42              |
| 35:BA:598:G:C5'     | 48:BP:15:ARG:HB3   | 2.47                     | 0.42              |
| 48:BP:35:HIS:O      | 48:BP:36:LYS:HB2   | 2.19                     | 0.42              |
| 48:BP:97:PRO:O      | 48:BP:98:GLU:CB    | 2.65                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 57:BY:2:ARG:C     | 57:BY:4:LYS:H     | 2.23                     | 0.42              |
| 1:AA:112:G:H2'    | 1:AA:113:G:C5'    | 2.25                     | 0.42              |
| 1:AA:1158:C:O2    | 1:AA:1158:C:O2'   | 2.36                     | 0.42              |
| 1:AA:1193:G:H2'   | 1:AA:1194:U:H5'   | 2.00                     | 0.42              |
| 1:AA:1385:G:N2    | 1:AA:1386:G:N3    | 2.67                     | 0.42              |
| 1:AA:203:U:OP2    | 1:AA:203:U:C6     | 2.72                     | 0.42              |
| 1:AA:264:U:HO2'   | 1:AA:265:G:H5'    | 1.77                     | 0.42              |
| 1:AA:370:C:C2     | 1:AA:392:G:N2     | 2.87                     | 0.42              |
| 1:AA:417:C:O2'    | 1:AA:418:C:H5'    | 2.19                     | 0.42              |
| 1:AA:560:U:O5'    | 1:AA:560:U:H6     | 2.03                     | 0.42              |
| 1:AA:924:C:H2'    | 1:AA:925:G:C8     | 2.54                     | 0.42              |
| 3:AC:20:SER:HB3   | 3:AC:40:ARG:HH22  | 1.84                     | 0.42              |
| 4:AD:3:ARG:NH2    | 4:AD:5:ILE:HG12   | 2.25                     | 0.42              |
| 6:AF:3:ARG:HD3    | 6:AF:64:GLN:NE2   | 2.35                     | 0.42              |
| 6:AF:45:LEU:HD21  | 6:AF:57:GLN:HE22  | 1.85                     | 0.42              |
| 6:AF:69:GLU:HG2   | 6:AF:70:ASP:N     | 2.34                     | 0.42              |
| 9:AI:95:LYS:NZ    | 9:AI:96:LEU:CD1   | 2.82                     | 0.42              |
| 12:AL:34:ARG:O    | 12:AL:61:THR:HG23 | 2.19                     | 0.42              |
| 13:AM:97:PRO:CA   | 13:AM:110:ARG:HD3 | 2.49                     | 0.42              |
| 13:AM:28:ALA:O    | 13:AM:29:ARG:C    | 2.56                     | 0.42              |
| 18:AR:31:LEU:H    | 18:AR:31:LEU:HD23 | 1.84                     | 0.42              |
| 1:AA:1286:A:C2    | 21:AU:22:ARG:NH2  | 2.88                     | 0.42              |
| 22:AV:47:U:C6     | 22:AV:47:U:O5'    | 2.59                     | 0.42              |
| 1:AA:1498:U:O2'   | 23:AX:16:U:O3'    | 2.37                     | 0.42              |
| 25:B0:10:THR:CG2  | 25:B0:11:ARG:N    | 2.70                     | 0.42              |
| 26:B1:5:CYS:C     | 26:B1:7:ILE:H     | 2.22                     | 0.42              |
| 27:B2:43:GLN:HB2  | 27:B2:44:LEU:H    | 1.58                     | 0.42              |
| 29:B4:21:VAL:HG22 | 29:B4:35:VAL:HG21 | 2.02                     | 0.42              |
| 35:BA:1084:A:N7   | 35:BA:1085:A:C4   | 2.88                     | 0.42              |
| 35:BA:1104:C:O2'  | 35:BA:1105:U:C5'  | 2.66                     | 0.42              |
| 35:BA:1510:G:H2'  | 35:BA:1511:C:C6   | 2.54                     | 0.42              |
| 35:BA:1770:G:C5   | 35:BA:1771:C:C4   | 3.07                     | 0.42              |
| 35:BA:2153:G:N2   | 35:BA:2154:G:H1'  | 2.34                     | 0.42              |
| 35:BA:921:G:H4'   | 35:BA:2269:A:C5   | 2.54                     | 0.42              |
| 35:BA:2335:A:O2'  | 35:BA:2336:A:H5'' | 2.19                     | 0.42              |
| 35:BA:248:G:H5''  | 35:BA:386:G:N2    | 2.34                     | 0.42              |
| 35:BA:2693:A:H2'  | 35:BA:2694:G:H8   | 1.84                     | 0.42              |
| 35:BA:2774:C:H2'  | 35:BA:2775:A:O4'  | 2.19                     | 0.42              |
| 35:BA:376:C:H2'   | 35:BA:377:C:C6    | 2.54                     | 0.42              |
| 35:BA:45:C:N4     | 35:BA:47:C:H41    | 2.17                     | 0.42              |
| 35:BA:531:C:OP1   | 35:BA:561:G:N1    | 2.48                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:580:C:H2'    | 35:BA:581:C:C6     | 2.54                     | 0.42              |
| 35:BA:868:U:C4     | 35:BA:869:G:N7     | 2.87                     | 0.42              |
| 35:BA:882:G:H2'    | 35:BA:883:G:C8     | 2.43                     | 0.42              |
| 35:BA:896:A:C2     | 58:BZ:177:PRO:HD2  | 2.54                     | 0.42              |
| 35:BA:992:C:OP1    | 54:BV:74:LYS:NZ    | 2.51                     | 0.42              |
| 36:BB:38:C:O2      | 36:BB:48:A:H1'     | 2.19                     | 0.42              |
| 36:BB:68:C:O2'     | 36:BB:69:G:H5'     | 2.19                     | 0.42              |
| 35:BA:1800:C:H5'   | 38:BD:147:LEU:CD2  | 2.49                     | 0.42              |
| 41:BG:104:GLU:HA   | 41:BG:107:LEU:CB   | 2.50                     | 0.42              |
| 41:BG:137:GLU:CG   | 41:BG:155:MET:N    | 2.82                     | 0.42              |
| 41:BG:164:GLU:O    | 41:BG:165:THR:C    | 2.58                     | 0.42              |
| 41:BG:170:ARG:NE   | 41:BG:180:PHE:HE2  | 2.17                     | 0.42              |
| 45:BL:106:UNK:O    | 45:BL:107:UNK:C    | 2.68                     | 0.42              |
| 47:BO:20:MET:CE    | 47:BO:44:LYS:HE3   | 2.48                     | 0.42              |
| 48:BP:124:LYS:HE3  | 48:BP:142:GLY:O    | 2.20                     | 0.42              |
| 50:BR:116:LEU:HA   | 50:BR:116:LEU:HD23 | 1.67                     | 0.42              |
| 51:BS:42:ASP:C     | 51:BS:44:LYS:N     | 2.71                     | 0.42              |
| 51:BS:53:SER:C     | 51:BS:55:ALA:N     | 2.73                     | 0.42              |
| 54:BV:47:VAL:HG12  | 54:BV:52:VAL:CB    | 2.49                     | 0.42              |
| 54:BV:29:PRO:CA    | 54:BV:61:VAL:HG23  | 2.43                     | 0.42              |
| 56:BX:23:GLU:O     | 56:BX:25:LYS:N     | 2.45                     | 0.42              |
| 56:BX:22:ALA:HB3   | 56:BX:23:GLU:OE2   | 2.19                     | 0.42              |
| 56:BX:52:VAL:O     | 56:BX:52:VAL:HG12  | 2.20                     | 0.42              |
| 58:BZ:102:LEU:HD21 | 58:BZ:124:ILE:CD1  | 2.49                     | 0.42              |
| 58:BZ:183:LEU:C    | 58:BZ:183:LEU:HD12 | 2.36                     | 0.42              |
| 49:BQ:141:GLN:NE2  | 58:BZ:72:ARG:NE    | 2.67                     | 0.42              |
| 1:AA:1096:C:O2'    | 1:AA:1097:C:H5'    | 2.20                     | 0.42              |
| 1:AA:1389:C:H6     | 1:AA:1389:C:O5'    | 2.03                     | 0.42              |
| 1:AA:1403:C:O5'    | 1:AA:1403:C:H6     | 2.03                     | 0.42              |
| 1:AA:1440:C:O2'    | 1:AA:1441:G:H5'    | 2.19                     | 0.42              |
| 1:AA:45:U:H2'      | 1:AA:46:G:C8       | 2.54                     | 0.42              |
| 1:AA:862:C:C3'     | 1:AA:863:U:H5'     | 2.45                     | 0.42              |
| 2:AB:204:ASN:ND2   | 2:AB:204:ASN:C     | 2.72                     | 0.42              |
| 4:AD:191:ARG:HD3   | 4:AD:200:GLU:OE1   | 2.19                     | 0.42              |
| 4:AD:18:LYS:HG3    | 4:AD:33:MET:HG3    | 2.00                     | 0.42              |
| 5:AE:145:LYS:HA    | 8:AH:107:LEU:HD22  | 2.02                     | 0.42              |
| 7:AG:31:MET:SD     | 7:AG:36:LYS:HB2    | 2.59                     | 0.42              |
| 7:AG:33:ASP:C      | 7:AG:35:LYS:N      | 2.72                     | 0.42              |
| 9:AI:47:LEU:CD1    | 9:AI:47:LEU:N      | 2.82                     | 0.42              |
| 10:AJ:9:ARG:HH22   | 10:AJ:97:GLU:HG3   | 1.84                     | 0.42              |
| 12:AL:111:LYS:O    | 12:AL:112:ASP:HB2  | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:16:ASP:OD1   | 13:AM:16:ASP:N     | 2.53                     | 0.42              |
| 13:AM:23:TYR:CD2   | 13:AM:70:LEU:HD13  | 2.55                     | 0.42              |
| 14:AN:41:ARG:NH1   | 14:AN:42:ILE:HD13  | 2.34                     | 0.42              |
| 15:AO:74:ASP:HB3   | 15:AO:77:ARG:HG2   | 2.00                     | 0.42              |
| 17:AQ:68:ARG:N     | 17:AQ:70:ARG:NH1   | 2.64                     | 0.42              |
| 24:AY:109:ASP:O    | 24:AY:111:SER:N    | 2.53                     | 0.42              |
| 24:AY:203:GLU:O    | 24:AY:204:GLU:C    | 2.57                     | 0.42              |
| 24:AY:238:THR:HG22 | 24:AY:241:GLU:CD   | 2.40                     | 0.42              |
| 24:AY:517:LEU:HD13 | 24:AY:563:ILE:CA   | 2.50                     | 0.42              |
| 24:AY:57:GLN:NE2   | 24:AY:464:ASP:OD1  | 2.52                     | 0.42              |
| 24:AY:621:ILE:CG1  | 24:AY:643:ILE:HD13 | 2.49                     | 0.42              |
| 24:AY:87:HIS:HE2   | 35:BA:2662:A:P     | 2.42                     | 0.42              |
| 25:B0:53:MET:SD    | 25:B0:57:PHE:HB3   | 2.59                     | 0.42              |
| 26:B1:58:ILE:HD11  | 26:B1:90:ILE:HB    | 2.01                     | 0.42              |
| 27:B2:2:LYS:HE3    | 27:B2:52:ASP:CG    | 2.39                     | 0.42              |
| 31:B6:17:LYS:O     | 31:B6:18:ARG:HD2   | 2.20                     | 0.42              |
| 34:B9:35:ARG:HD3   | 35:BA:2742:C:OP1   | 2.20                     | 0.42              |
| 35:BA:1027:A:N6    | 35:BA:1126:A:N9    | 2.68                     | 0.42              |
| 35:BA:1564:C:O2'   | 35:BA:1565:C:H5'   | 2.19                     | 0.42              |
| 35:BA:1787:A:C2    | 35:BA:1788:C:C5    | 3.08                     | 0.42              |
| 35:BA:2000:G:H21   | 35:BA:2001:A:C1'   | 2.32                     | 0.42              |
| 35:BA:2009:G:N3    | 35:BA:2010:G:C8    | 2.88                     | 0.42              |
| 35:BA:2823:A:OP1   | 39:BE:113:PHE:HB2  | 2.19                     | 0.42              |
| 35:BA:299:A:C5     | 35:BA:322:A:C2     | 3.07                     | 0.42              |
| 35:BA:310:A:P      | 57:BY:18:GLY:HA2   | 2.59                     | 0.42              |
| 35:BA:603:A:N7     | 35:BA:655:A:C5     | 2.87                     | 0.42              |
| 35:BA:811:U:P      | 48:BP:33:ARG:NH1   | 2.92                     | 0.42              |
| 37:BC:89:GLU:O     | 37:BC:91:GLY:N     | 2.51                     | 0.42              |
| 38:BD:65:ILE:HD13  | 38:BD:65:ILE:C     | 2.39                     | 0.42              |
| 40:BF:110:LEU:HD21 | 40:BF:181:LEU:HG   | 2.01                     | 0.42              |
| 40:BF:28:ILE:H     | 40:BF:28:ILE:CD1   | 2.32                     | 0.42              |
| 41:BG:138:GLN:C    | 41:BG:140:ILE:H    | 2.23                     | 0.42              |
| 41:BG:144:ILE:CG2  | 41:BG:145:THR:H    | 2.30                     | 0.42              |
| 35:BA:2310:A:C5    | 41:BG:75:LYS:HE2   | 2.53                     | 0.42              |
| 41:BG:38:VAL:CA    | 41:BG:93:THR:HA    | 2.41                     | 0.42              |
| 41:BG:96:ARG:O     | 41:BG:97:ASP:C     | 2.58                     | 0.42              |
| 45:BL:106:UNK:C    | 45:BL:108:UNK:N    | 2.81                     | 0.42              |
| 48:BP:115:LEU:CB   | 48:BP:131:SER:OG   | 2.67                     | 0.42              |
| 49:BQ:56:ARG:NH1   | 49:BQ:56:ARG:CG    | 2.76                     | 0.42              |
| 49:BQ:6:ARG:O      | 49:BQ:7:MET:HG3    | 2.19                     | 0.42              |
| 50:BR:107:ASP:C    | 50:BR:107:ASP:OD1  | 2.56                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:BU:91:ASP:O    | 53:BU:95:LEU:HB2   | 2.19                     | 0.42              |
| 56:BX:28:PHE:CE2  | 56:BX:92:LEU:HD11  | 2.54                     | 0.42              |
| 1:AA:1010:G:O2'   | 1:AA:1011:G:H5'    | 2.19                     | 0.42              |
| 1:AA:1287:A:C6    | 1:AA:1288:A:N6     | 2.88                     | 0.42              |
| 1:AA:1368:G:OP1   | 10:AJ:62:HIS:NE2   | 2.44                     | 0.42              |
| 1:AA:1393:U:HO2'  | 1:AA:1501:C:HO2'   | 1.67                     | 0.42              |
| 1:AA:563:A:N3     | 1:AA:563:A:C3'     | 2.83                     | 0.42              |
| 1:AA:867:G:O2'    | 1:AA:868:C:H5'     | 2.19                     | 0.42              |
| 1:AA:954:G:O2'    | 1:AA:955:U:H5'     | 2.19                     | 0.42              |
| 1:AA:980:C:C5'    | 1:AA:980:C:H6      | 2.20                     | 0.42              |
| 2:AB:7:VAL:O      | 2:AB:11:LEU:HD12   | 2.19                     | 0.42              |
| 2:AB:72:GLY:O     | 2:AB:94:ASN:HA     | 2.19                     | 0.42              |
| 3:AC:123:GLN:HE21 | 3:AC:123:GLN:CA    | 2.33                     | 0.42              |
| 3:AC:31:HIS:O     | 3:AC:33:LEU:N      | 2.52                     | 0.42              |
| 5:AE:120:THR:HG22 | 5:AE:121:LYS:N     | 2.35                     | 0.42              |
| 7:AG:71:PRO:HD3   | 7:AG:103:TRP:HZ3   | 1.82                     | 0.42              |
| 7:AG:74:GLU:HG2   | 7:AG:91:VAL:CG2    | 2.47                     | 0.42              |
| 11:AK:56:GLY:O    | 11:AK:89:ALA:CB    | 2.67                     | 0.42              |
| 12:AL:20:LYS:N    | 12:AL:20:LYS:CD    | 2.83                     | 0.42              |
| 19:AS:29:ARG:O    | 19:AS:31:ILE:HG22  | 2.18                     | 0.42              |
| 24:AY:126:GLU:HG2 | 24:AY:132:ARG:NH2  | 2.29                     | 0.42              |
| 24:AY:113:GLY:HA3 | 24:AY:152:THR:HG21 | 2.02                     | 0.42              |
| 25:B0:5:LYS:O     | 25:B0:6:GLY:C      | 2.58                     | 0.42              |
| 26:B1:25:LYS:HB2  | 26:B1:25:LYS:HE3   | 1.56                     | 0.42              |
| 26:B1:3:LYS:O     | 26:B1:12:PRO:HD3   | 2.20                     | 0.42              |
| 26:B1:52:ARG:O    | 26:B1:53:VAL:O     | 2.37                     | 0.42              |
| 28:B3:9:VAL:HG21  | 28:B3:55:ARG:HD2   | 2.01                     | 0.42              |
| 19:AS:20:LEU:HD13 | 29:B4:61:ARG:NH2   | 2.33                     | 0.42              |
| 31:B6:45:LYS:C    | 31:B6:46:HIS:ND1   | 2.73                     | 0.42              |
| 35:BA:1022:G:C5   | 35:BA:1141:U:O4    | 2.73                     | 0.42              |
| 35:BA:1144:G:C6   | 35:BA:1145:C:C4    | 3.08                     | 0.42              |
| 35:BA:1348:G:H2'  | 35:BA:1349:A:C5'   | 2.47                     | 0.42              |
| 35:BA:1530:C:H2'  | 35:BA:1531:C:C6    | 2.55                     | 0.42              |
| 35:BA:1817:G:H2'  | 35:BA:1818:U:C5'   | 2.31                     | 0.42              |
| 35:BA:192:C:C5    | 35:BA:193:U:C6     | 3.07                     | 0.42              |
| 35:BA:1936:A:OP2  | 35:BA:1961:C:N4    | 2.51                     | 0.42              |
| 35:BA:2174:C:C3'  | 35:BA:2175:C:H5'   | 2.49                     | 0.42              |
| 35:BA:328:U:H2'   | 35:BA:329:G:OP1    | 2.19                     | 0.42              |
| 35:BA:646:A:H2'   | 35:BA:647:G:O4'    | 2.19                     | 0.42              |
| 35:BA:697:C:H2'   | 35:BA:698:C:C5'    | 2.45                     | 0.42              |
| 35:BA:999:U:H5''  | 35:BA:1154:G:O6    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BB:106:G:H2'    | 36:BB:107:G:H8     | 1.84                     | 0.42              |
| 36:BB:66:A:O2'     | 36:BB:67:G:P       | 2.76                     | 0.42              |
| 38:BD:105:ILE:HD12 | 38:BD:105:ILE:HA   | 1.80                     | 0.42              |
| 38:BD:70:TRP:O     | 38:BD:73:VAL:HG23  | 2.19                     | 0.42              |
| 40:BF:4:VAL:H      | 40:BF:24:LEU:HD12  | 1.84                     | 0.42              |
| 41:BG:140:ILE:O    | 41:BG:141:PHE:O    | 2.37                     | 0.42              |
| 41:BG:50:ALA:C     | 41:BG:52:ILE:H     | 2.23                     | 0.42              |
| 41:BG:93:THR:CG2   | 41:BG:94:LEU:H     | 2.29                     | 0.42              |
| 47:BO:104:ARG:NH1  | 47:BO:107:ARG:NH1  | 2.60                     | 0.42              |
| 35:BA:2563:U:H4'   | 47:BO:28:SER:HA    | 2.00                     | 0.42              |
| 47:BO:35:VAL:CG2   | 47:BO:69:ILE:HD11  | 2.48                     | 0.42              |
| 35:BA:943:U:OP2    | 48:BP:38:GLN:NE2   | 2.52                     | 0.42              |
| 51:BS:92:TYR:CD1   | 51:BS:93:LYS:N     | 2.87                     | 0.42              |
| 52:BT:58:ASN:HD22  | 52:BT:58:ASN:N     | 2.10                     | 0.42              |
| 55:BW:12:ILE:HD13  | 55:BW:17:VAL:HG22  | 2.02                     | 0.42              |
| 57:BY:97:ARG:O     | 57:BY:98:VAL:CG2   | 2.67                     | 0.42              |
| 58:BZ:5:LEU:HD11   | 58:BZ:39:VAL:HB    | 2.02                     | 0.42              |
| 1:AA:1116:C:O2'    | 1:AA:1117:G:H5''   | 2.19                     | 0.42              |
| 1:AA:1304:G:H1'    | 1:AA:1333:A:N6     | 2.32                     | 0.42              |
| 1:AA:22:G:H4'      | 1:AA:885:G:C8      | 2.55                     | 0.42              |
| 1:AA:38:G:O2'      | 1:AA:39:G:C5'      | 2.68                     | 0.42              |
| 1:AA:507:C:C2'     | 1:AA:508:C:OP1     | 2.68                     | 0.42              |
| 2:AB:51:LEU:CD2    | 2:AB:201:ILE:HD12  | 2.49                     | 0.42              |
| 3:AC:84:ILE:C      | 3:AC:86:VAL:H      | 2.23                     | 0.42              |
| 7:AG:125:MET:O     | 7:AG:128:ALA:CB    | 2.65                     | 0.42              |
| 8:AH:104:ARG:O     | 8:AH:105:ARG:C     | 2.58                     | 0.42              |
| 14:AN:24:CYS:HB2   | 14:AN:40:CYS:HB3   | 2.01                     | 0.42              |
| 14:AN:26:ARG:HB3   | 14:AN:43:CYS:SG    | 2.59                     | 0.42              |
| 15:AO:66:LEU:HD12  | 15:AO:66:LEU:HA    | 1.88                     | 0.42              |
| 16:AP:52:ASP:O     | 16:AP:53:VAL:C     | 2.57                     | 0.42              |
| 24:AY:150:ILE:HD11 | 24:AY:163:VAL:HG22 | 2.01                     | 0.42              |
| 24:AY:237:PRO:HB2  | 24:AY:242:LEU:HG   | 2.02                     | 0.42              |
| 24:AY:7:TYR:CZ     | 24:AY:370:LYS:HB2  | 2.55                     | 0.42              |
| 24:AY:5:VAL:C      | 24:AY:7:TYR:N      | 2.72                     | 0.42              |
| 28:B3:1:MET:CG     | 28:B3:2:PRO:HD2    | 2.49                     | 0.42              |
| 29:B4:33:VAL:CG1   | 29:B4:34:GLU:H     | 2.22                     | 0.42              |
| 35:BA:1203:G:H3'   | 35:BA:1204:A:H5''  | 2.01                     | 0.42              |
| 35:BA:1820:U:HO2'  | 35:BA:1821:A:P     | 2.42                     | 0.42              |
| 35:BA:2203:U:O3'   | 35:BA:2205:C:OP1   | 2.38                     | 0.42              |
| 35:BA:221:A:H4'    | 35:BA:222:A:O5'    | 2.20                     | 0.42              |
| 35:BA:2241:A:H2'   | 35:BA:2242:G:C8    | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2722:G:H2'   | 35:BA:2723:C:C6    | 2.55                     | 0.42              |
| 35:BA:2789:C:H5'   | 35:BA:2790:A:OP1   | 2.20                     | 0.42              |
| 35:BA:2808:U:H5    | 35:BA:2891:G:C5    | 2.37                     | 0.42              |
| 35:BA:359:A:H2'    | 35:BA:360:G:O4'    | 2.20                     | 0.42              |
| 35:BA:54:G:C2'     | 35:BA:55:G:O5'     | 2.67                     | 0.42              |
| 35:BA:554:U:C2'    | 35:BA:555:U:H5'    | 2.50                     | 0.42              |
| 35:BA:607:U:H6     | 35:BA:607:U:H3'    | 1.85                     | 0.42              |
| 35:BA:752:A:HO2'   | 35:BA:753:C:P      | 2.39                     | 0.42              |
| 35:BA:922:U:H2'    | 35:BA:923:C:C6     | 2.55                     | 0.42              |
| 37:BC:103:LYS:HZ2  | 37:BC:103:LYS:CB   | 2.32                     | 0.42              |
| 37:BC:73:VAL:CG1   | 37:BC:74:ARG:H     | 2.33                     | 0.42              |
| 37:BC:89:GLU:C     | 37:BC:91:GLY:N     | 2.72                     | 0.42              |
| 38:BD:43:ARG:HB2   | 38:BD:54:ARG:HB2   | 2.01                     | 0.42              |
| 38:BD:30:GLU:CG    | 38:BD:63:ARG:CZ    | 2.87                     | 0.42              |
| 38:BD:7:LYS:O      | 38:BD:9:TYR:N      | 2.50                     | 0.42              |
| 41:BG:67:LYS:HA    | 41:BG:68:PRO:HD3   | 1.78                     | 0.42              |
| 44:BK:70:UNK:O     | 44:BK:71:UNK:CB    | 2.68                     | 0.42              |
| 52:BT:105:LEU:HD22 | 52:BT:109:GLU:OE1  | 2.20                     | 0.42              |
| 52:BT:93:ARG:HD2   | 52:BT:93:ARG:HA    | 1.79                     | 0.42              |
| 55:BW:24:ILE:O     | 55:BW:71:VAL:CG2   | 2.67                     | 0.42              |
| 1:AA:1053:G:O6     | 1:AA:1199:U:H2'    | 2.20                     | 0.42              |
| 1:AA:190:U:O2'     | 1:AA:191:G:H5'     | 2.19                     | 0.42              |
| 1:AA:38:G:O2'      | 1:AA:39:G:H5''     | 2.20                     | 0.42              |
| 1:AA:39:G:N9       | 1:AA:498:U:C4      | 2.59                     | 0.42              |
| 1:AA:490:G:C2      | 1:AA:491:G:C5      | 3.07                     | 0.42              |
| 1:AA:796:C:HO2'    | 1:AA:797:C:H5'     | 1.77                     | 0.42              |
| 1:AA:936:C:C2'     | 1:AA:937:A:O5'     | 2.68                     | 0.42              |
| 2:AB:51:LEU:HD23   | 2:AB:201:ILE:HD12  | 2.01                     | 0.42              |
| 2:AB:15:VAL:CG2    | 2:AB:209:ARG:HH21  | 2.14                     | 0.42              |
| 2:AB:73:THR:O      | 2:AB:78:GLN:HG3    | 2.20                     | 0.42              |
| 3:AC:129:ALA:CB    | 3:AC:132:ARG:HG3   | 2.47                     | 0.42              |
| 4:AD:120:LEU:C     | 4:AD:126:ILE:HD13  | 2.40                     | 0.42              |
| 4:AD:39:PRO:HB2    | 4:AD:44:GLY:HA2    | 2.02                     | 0.42              |
| 4:AD:57:ARG:HB3    | 4:AD:206:PHE:HB2   | 2.01                     | 0.42              |
| 5:AE:36:ASP:O      | 5:AE:37:ARG:HB2    | 2.20                     | 0.42              |
| 7:AG:138:LYS:HD3   | 7:AG:138:LYS:C     | 2.40                     | 0.42              |
| 20:AT:41:ILE:HG12  | 20:AT:41:ILE:H     | 1.58                     | 0.42              |
| 24:AY:179:ASP:OD1  | 24:AY:181:LEU:HB3  | 2.20                     | 0.42              |
| 24:AY:210:ARG:CG   | 24:AY:210:ARG:HH11 | 2.31                     | 0.42              |
| 24:AY:218:GLU:OE2  | 45:BL:83:UNK:CB    | 2.68                     | 0.42              |
| 24:AY:494:GLU:O    | 24:AY:494:GLU:HG3  | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:556:ILE:HG13 | 24:AY:558:PHE:CD1  | 2.55                     | 0.42              |
| 24:AY:614:GLU:HG3  | 24:AY:617:MET:CE   | 2.48                     | 0.42              |
| 24:AY:605:ILE:HD13 | 24:AY:677:GLN:HG2  | 2.02                     | 0.42              |
| 25:B0:7:LEU:O      | 25:B0:8:GLY:O      | 2.37                     | 0.42              |
| 29:B4:12:ALA:CA    | 29:B4:24:THR:HG22  | 2.25                     | 0.42              |
| 33:B8:5:LYS:HG2    | 35:BA:242:G:C8     | 2.54                     | 0.42              |
| 35:BA:1060:U:C4    | 35:BA:1062:G:H4'   | 2.55                     | 0.42              |
| 35:BA:1027:A:N6    | 35:BA:1126:A:C1'   | 2.83                     | 0.42              |
| 35:BA:1213:A:C2'   | 35:BA:1214:A:H5'   | 2.50                     | 0.42              |
| 35:BA:1221:C:C2    | 35:BA:1221(A):C:C5 | 3.06                     | 0.42              |
| 35:BA:1541:G:O2'   | 35:BA:1542:A:P     | 2.77                     | 0.42              |
| 35:BA:1856:G:C2    | 35:BA:1887:C:C2    | 3.08                     | 0.42              |
| 35:BA:1678:G:H21   | 35:BA:1989:G:N2    | 2.06                     | 0.42              |
| 35:BA:2039:C:H2'   | 35:BA:2040:C:H6    | 1.85                     | 0.42              |
| 35:BA:526:A:O2'    | 35:BA:2043:C:H2'   | 2.14                     | 0.42              |
| 25:B0:3:HIS:HB2    | 35:BA:2494:G:H5'   | 2.01                     | 0.42              |
| 35:BA:2810:A:H2'   | 39:BE:61:ARG:NH2   | 2.35                     | 0.42              |
| 35:BA:36:G:N2      | 35:BA:444:C:O2     | 2.45                     | 0.42              |
| 35:BA:861:A:H2'    | 35:BA:862:G:O4'    | 2.20                     | 0.42              |
| 36:BB:13:A:O2'     | 36:BB:15:A:H5''    | 2.19                     | 0.42              |
| 37:BC:97:GLY:O     | 37:BC:98:GLU:C     | 2.58                     | 0.42              |
| 38:BD:112:GLN:HB2  | 38:BD:115:GLN:NE2  | 2.35                     | 0.42              |
| 39:BE:67:PHE:CE1   | 39:BE:69:LYS:HE3   | 2.55                     | 0.42              |
| 41:BG:64:THR:HA    | 41:BG:102:PHE:CD1  | 2.54                     | 0.42              |
| 41:BG:22:ARG:O     | 41:BG:23:PHE:CG    | 2.72                     | 0.42              |
| 41:BG:40:ASN:HA    | 41:BG:91:ARG:HB2   | 2.01                     | 0.42              |
| 41:BG:66:GLN:OE1   | 41:BG:94:LEU:CG    | 2.61                     | 0.42              |
| 42:BH:98:LEU:HB2   | 42:BH:125:VAL:CG2  | 2.50                     | 0.42              |
| 48:BP:78:PRO:CA    | 48:BP:110:TYR:HE2  | 2.31                     | 0.42              |
| 51:BS:57:LYS:HD2   | 51:BS:58:LEU:N     | 2.35                     | 0.42              |
| 51:BS:61:ASN:O     | 51:BS:65:VAL:HG23  | 2.20                     | 0.42              |
| 51:BS:90:GLY:C     | 51:BS:92:TYR:H     | 2.22                     | 0.42              |
| 52:BT:126:ALA:C    | 52:BT:128:GLU:N    | 2.69                     | 0.42              |
| 54:BV:39:LEU:CD1   | 54:BV:51:VAL:HA    | 2.50                     | 0.42              |
| 54:BV:66:ARG:O     | 54:BV:67:GLY:O     | 2.38                     | 0.42              |
| 57:BY:88:LYS:CB    | 57:BY:91:GLU:HB2   | 2.49                     | 0.42              |
| 1:AA:1134:G:N2     | 1:AA:1141:C:C2     | 2.88                     | 0.42              |
| 1:AA:1279:A:H2     | 10:AJ:43:ARG:HH12  | 1.68                     | 0.42              |
| 1:AA:347:G:H21     | 1:AA:348:G:H1'     | 1.85                     | 0.42              |
| 1:AA:683:G:C5      | 1:AA:684:A:C5      | 3.07                     | 0.42              |
| 3:AC:22:TRP:CE2    | 14:AN:54:PRO:CG    | 2.94                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AC:71:ALA:HB2   | 3:AC:115:LEU:CD2   | 2.47                     | 0.42              |
| 5:AE:92:LYS:HA    | 5:AE:93:PRO:HD3    | 1.95                     | 0.42              |
| 7:AG:86:GLN:O     | 7:AG:87:VAL:CG1    | 2.68                     | 0.42              |
| 10:AJ:54:PHE:CZ   | 10:AJ:55:LYS:CE    | 3.03                     | 0.42              |
| 11:AK:81:ASP:OD1  | 11:AK:107:SER:OG   | 2.34                     | 0.42              |
| 1:AA:1316:G:O2'   | 14:AN:18:VAL:HG11  | 2.19                     | 0.42              |
| 15:AO:56:LEU:HD13 | 15:AO:56:LEU:O     | 2.20                     | 0.42              |
| 15:AO:75:PRO:O    | 15:AO:78:TYR:HB3   | 2.20                     | 0.42              |
| 19:AS:88:LYS:O    | 19:AS:90:THR:N     | 2.53                     | 0.42              |
| 24:AY:15:ILE:HG22 | 24:AY:103:GLY:CA   | 2.50                     | 0.42              |
| 24:AY:315:LYS:O   | 24:AY:316:ILE:HD13 | 2.19                     | 0.42              |
| 24:AY:515:GLU:OE1 | 24:AY:515:GLU:N    | 2.53                     | 0.42              |
| 26:B1:78:LYS:HB3  | 26:B1:78:LYS:HE2   | 1.68                     | 0.42              |
| 29:B4:30:GLU:CG   | 29:B4:31:ILE:N     | 2.81                     | 0.42              |
| 30:B5:10:LYS:HG3  | 35:BA:1263:U:C1'   | 2.50                     | 0.42              |
| 35:BA:1036:G:N1   | 35:BA:1120:G:C5    | 2.88                     | 0.42              |
| 35:BA:1558:A:H4'  | 35:BA:1559:G:H2'   | 2.02                     | 0.42              |
| 35:BA:1625:C:C2'  | 35:BA:1626:G:H5'   | 2.50                     | 0.42              |
| 35:BA:1823:G:O2'  | 35:BA:1824:G:H5'   | 2.20                     | 0.42              |
| 35:BA:17:G:O2'    | 35:BA:18:C:H5'     | 2.20                     | 0.42              |
| 35:BA:2307:G:N3   | 35:BA:2307:G:H3'   | 2.35                     | 0.42              |
| 35:BA:2567:G:H2'  | 35:BA:2568:C:H6    | 1.84                     | 0.42              |
| 35:BA:548:A:C2'   | 35:BA:549:G:H5'    | 2.49                     | 0.42              |
| 35:BA:753:C:H2'   | 35:BA:754:C:C6     | 2.55                     | 0.42              |
| 35:BA:92:A:C2     | 35:BA:93:G:H1'     | 2.55                     | 0.42              |
| 37:BC:42:VAL:O    | 37:BC:216:THR:C    | 2.59                     | 0.42              |
| 37:BC:48:LEU:CD2  | 37:BC:59:VAL:HG21  | 2.50                     | 0.42              |
| 39:BE:170:LEU:N   | 39:BE:170:LEU:HD12 | 2.34                     | 0.42              |
| 39:BE:201:THR:OG1 | 39:BE:202:LYS:N    | 2.52                     | 0.42              |
| 39:BE:92:THR:O    | 39:BE:95:ILE:HG12  | 2.20                     | 0.42              |
| 40:BF:10:PRO:HD2  | 40:BF:13:SER:O     | 2.19                     | 0.42              |
| 40:BF:7:TYR:CE1   | 40:BF:196:LEU:HD11 | 2.55                     | 0.42              |
| 41:BG:7:LEU:HD11  | 41:BG:176:LEU:HD21 | 2.02                     | 0.42              |
| 41:BG:7:LEU:HD12  | 41:BG:104:GLU:HG3  | 2.01                     | 0.42              |
| 48:BP:88:LEU:HD21 | 48:BP:125:VAL:HG21 | 2.02                     | 0.42              |
| 50:BR:104:ARG:HD2 | 50:BR:109:ALA:HB3  | 2.02                     | 0.42              |
| 50:BR:116:LEU:O   | 50:BR:117:VAL:HG12 | 2.20                     | 0.42              |
| 52:BT:90:GLN:HB3  | 52:BT:121:ILE:CG1  | 2.50                     | 0.42              |
| 53:BU:59:ARG:NH1  | 53:BU:59:ARG:CG    | 2.81                     | 0.42              |
| 53:BU:84:LYS:HD2  | 53:BU:89:GLU:HG3   | 2.02                     | 0.42              |
| 56:BX:35:THR:HB   | 56:BX:38:GLU:HB2   | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1296:C:H4'    | 1:AA:1302:U:O4     | 2.20                     | 0.42              |
| 1:AA:1495:U:H2'    | 1:AA:1496:C:C6     | 2.55                     | 0.42              |
| 1:AA:240:C:H2'     | 1:AA:241:C:H6      | 1.85                     | 0.42              |
| 1:AA:368:U:C3'     | 1:AA:368:U:C6      | 3.03                     | 0.42              |
| 1:AA:495:A:O2'     | 1:AA:496:A:O5'     | 2.30                     | 0.42              |
| 1:AA:560:U:C4'     | 1:AA:561:U:C5'     | 2.76                     | 0.42              |
| 1:AA:663:A:C2'     | 1:AA:664:G:H5'     | 2.49                     | 0.42              |
| 1:AA:748:C:H1'     | 1:AA:749:C:C5      | 2.48                     | 0.42              |
| 2:AB:127:ILE:C     | 2:AB:129:GLU:H     | 2.23                     | 0.42              |
| 4:AD:81:GLU:OE2    | 4:AD:139:ARG:NH2   | 2.52                     | 0.42              |
| 5:AE:145:LYS:HD2   | 8:AH:107:LEU:CD2   | 2.50                     | 0.42              |
| 5:AE:38:GLN:HB3    | 5:AE:38:GLN:HE21   | 1.69                     | 0.42              |
| 14:AN:42:ILE:O     | 14:AN:46:GLU:HG3   | 2.20                     | 0.42              |
| 17:AQ:65:ILE:HG22  | 17:AQ:65:ILE:O     | 2.20                     | 0.42              |
| 17:AQ:67:LYS:CA    | 17:AQ:70:ARG:NH1   | 2.81                     | 0.42              |
| 24:AY:146:LEU:O    | 24:AY:146:LEU:HD23 | 2.19                     | 0.42              |
| 24:AY:403:GLU:HG3  | 24:AY:404:VAL:N    | 2.35                     | 0.42              |
| 24:AY:486:THR:HG21 | 24:AY:519:ARG:NH2  | 2.35                     | 0.42              |
| 25:B0:2:ALA:HB3    | 35:BA:2602:A:H61   | 1.85                     | 0.42              |
| 25:B0:78:TYR:O     | 25:B0:79:VAL:CG2   | 2.63                     | 0.42              |
| 30:B5:53:ALA:HA    | 30:B5:56:LYS:HZ2   | 1.73                     | 0.42              |
| 35:BA:1076:C:C5    | 35:BA:1077:A:N7    | 2.88                     | 0.42              |
| 35:BA:1902:C:H2'   | 35:BA:1903:G:O5'   | 2.19                     | 0.42              |
| 35:BA:2033:A:C4'   | 35:BA:2034:U:OP1   | 2.57                     | 0.42              |
| 35:BA:2177:C:N4    | 35:BA:2178:C:C4    | 2.87                     | 0.42              |
| 35:BA:2292:C:O2'   | 35:BA:2293:C:H5'   | 2.20                     | 0.42              |
| 25:B0:36:ILE:CD1   | 35:BA:2355:C:O4'   | 2.68                     | 0.42              |
| 35:BA:2615:U:H2'   | 35:BA:2616:C:C6    | 2.55                     | 0.42              |
| 35:BA:575:A:OP2    | 35:BA:2499:C:O2'   | 2.32                     | 0.42              |
| 35:BA:586:A:H2     | 35:BA:809:G:N3     | 2.18                     | 0.42              |
| 35:BA:66:C:O2'     | 35:BA:67:U:H5'     | 2.20                     | 0.42              |
| 35:BA:908:C:O2'    | 35:BA:909:A:H5'    | 2.20                     | 0.42              |
| 36:BB:13:A:HO2'    | 36:BB:15:A:H5''    | 1.85                     | 0.42              |
| 37:BC:6:LYS:N      | 37:BC:9:ARG:HH12   | 2.17                     | 0.42              |
| 38:BD:4:LYS:O      | 38:BD:17:THR:HA    | 2.19                     | 0.42              |
| 39:BE:167:VAL:CG2  | 39:BE:170:LEU:HD11 | 2.50                     | 0.42              |
| 39:BE:51:PHE:CG    | 39:BE:52:LEU:N     | 2.88                     | 0.42              |
| 40:BF:28:ILE:HD13  | 40:BF:28:ILE:H     | 1.85                     | 0.42              |
| 29:B4:22:ILE:CG1   | 41:BG:105:LYS:HD3  | 2.50                     | 0.42              |
| 41:BG:110:ALA:HB1  | 41:BG:142:PRO:CB   | 2.50                     | 0.42              |
| 36:BB:42:C:H41     | 41:BG:91:ARG:NH2   | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BH:98:LEU:HB2   | 42:BH:125:VAL:HG21 | 2.02                     | 0.42              |
| 42:BH:86:GLU:HB2   | 42:BH:132:ARG:HB3  | 2.02                     | 0.42              |
| 44:BK:63:UNK:O     | 44:BK:64:UNK:CB    | 2.67                     | 0.42              |
| 48:BP:47:ASP:CB    | 48:BP:49:ARG:N     | 2.74                     | 0.42              |
| 39:BE:111:ARG:HB3  | 50:BR:2:ARG:NH1    | 2.35                     | 0.42              |
| 50:BR:4:LEU:O      | 50:BR:4:LEU:CD2    | 2.68                     | 0.42              |
| 50:BR:79:LEU:HA    | 50:BR:83:ILE:HG12  | 2.02                     | 0.42              |
| 51:BS:87:PHE:O     | 51:BS:88:ASP:HB2   | 2.19                     | 0.42              |
| 53:BU:20:LEU:N     | 53:BU:20:LEU:HD22  | 2.32                     | 0.42              |
| 54:BV:19:LYS:HG2   | 54:BV:94:LEU:CB    | 2.42                     | 0.42              |
| 54:BV:19:LYS:HZ3   | 54:BV:20:LEU:C     | 2.23                     | 0.42              |
| 54:BV:47:VAL:HG12  | 54:BV:52:VAL:CA    | 2.49                     | 0.42              |
| 55:BW:36:LEU:CD2   | 55:BW:36:LEU:N     | 2.83                     | 0.42              |
| 58:BZ:155:LEU:H    | 58:BZ:155:LEU:HD23 | 1.85                     | 0.42              |
| 1:AA:1053:G:O2'    | 1:AA:1054:C:P      | 2.78                     | 0.41              |
| 1:AA:1151:A:O2'    | 1:AA:1152:A:OP2    | 2.30                     | 0.41              |
| 1:AA:1158:C:O2     | 1:AA:1158:C:H2'    | 2.17                     | 0.41              |
| 1:AA:131:C:H2'     | 1:AA:132:C:H6      | 1.85                     | 0.41              |
| 1:AA:222:U:H2'     | 1:AA:223:U:C6      | 2.55                     | 0.41              |
| 1:AA:748:C:O2'     | 1:AA:749:C:P       | 2.78                     | 0.41              |
| 1:AA:917:G:H2'     | 1:AA:918:A:C8      | 2.54                     | 0.41              |
| 1:AA:962:C:H2'     | 1:AA:963:G:O5'     | 2.20                     | 0.41              |
| 2:AB:39:ILE:O      | 2:AB:40:HIS:O      | 2.38                     | 0.41              |
| 2:AB:75:LYS:HB3    | 2:AB:76:GLN:HE21   | 1.85                     | 0.41              |
| 3:AC:120:VAL:O     | 3:AC:123:GLN:N     | 2.50                     | 0.41              |
| 5:AE:7:GLU:O       | 5:AE:8:GLU:HB3     | 2.19                     | 0.41              |
| 9:AI:17:VAL:HG23   | 9:AI:63:ILE:HG12   | 2.01                     | 0.41              |
| 11:AK:50:TYR:CD1   | 11:AK:54:ARG:HB3   | 2.54                     | 0.41              |
| 13:AM:52:GLU:HA    | 13:AM:55:ARG:HB3   | 2.02                     | 0.41              |
| 13:AM:67:GLU:CD    | 13:AM:71:ARG:HH21  | 2.23                     | 0.41              |
| 1:AA:979:C:O2      | 14:AN:19:ARG:HG2   | 2.20                     | 0.41              |
| 10:AJ:49:VAL:HG23  | 14:AN:41:ARG:HD3   | 2.01                     | 0.41              |
| 24:AY:328:ILE:HD11 | 24:AY:335:LEU:HD23 | 2.01                     | 0.41              |
| 24:AY:402:ILE:O    | 24:AY:403:GLU:CB   | 2.68                     | 0.41              |
| 24:AY:546:ILE:O    | 24:AY:550:MET:HB2  | 2.20                     | 0.41              |
| 24:AY:687:LEU:C    | 24:AY:688:ILE:HD12 | 2.40                     | 0.41              |
| 25:B0:67:VAL:HG12  | 25:B0:68:GLU:N     | 2.35                     | 0.41              |
| 26:B1:43:TYR:N     | 26:B1:43:TYR:CD1   | 2.87                     | 0.41              |
| 27:B2:22:GLU:O     | 27:B2:26:ARG:HD2   | 2.20                     | 0.41              |
| 27:B2:2:LYS:HA     | 27:B2:5:GLU:OE2    | 2.20                     | 0.41              |
| 29:B4:37:SER:O     | 29:B4:38:LYS:HB3   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 29:B4:46:GLN:HG3   | 29:B4:48:ARG:HD3    | 2.02                     | 0.41              |
| 29:B4:56:VAL:O     | 29:B4:58:ARG:N      | 2.53                     | 0.41              |
| 31:B6:25:LYS:HE2   | 33:B8:34:TRP:NE1    | 2.20                     | 0.41              |
| 35:BA:1038:C:C3'   | 35:BA:1039:G:C5'    | 2.90                     | 0.41              |
| 35:BA:1799:G:C2    | 35:BA:1800:C:C5     | 3.08                     | 0.41              |
| 35:BA:1822:G:C2'   | 35:BA:1823:G:C5'    | 2.96                     | 0.41              |
| 35:BA:1914:C:H3'   | 35:BA:1915:U:C6     | 2.55                     | 0.41              |
| 35:BA:2011:U:H2'   | 35:BA:2012:G:C5'    | 2.50                     | 0.41              |
| 35:BA:2171:A:O2'   | 35:BA:2172:U:O4'    | 2.26                     | 0.41              |
| 35:BA:2191:G:H2'   | 35:BA:2191:G:N3     | 2.35                     | 0.41              |
| 25:B0:39:ARG:NH2   | 35:BA:2355:C:O2     | 2.53                     | 0.41              |
| 35:BA:2363:C:C2'   | 35:BA:2364:C:H5'    | 2.42                     | 0.41              |
| 35:BA:2653:U:H3'   | 35:BA:2654:A:C8     | 2.55                     | 0.41              |
| 35:BA:2712(A):A:H8 | 35:BA:2712(A):A:O5' | 2.03                     | 0.41              |
| 35:BA:2785:C:H2'   | 35:BA:2786:U:C6     | 2.55                     | 0.41              |
| 35:BA:2788:C:H2'   | 35:BA:2789:C:O4'    | 2.20                     | 0.41              |
| 35:BA:28:A:N6      | 35:BA:512:G:O2'     | 2.53                     | 0.41              |
| 35:BA:654(F):C:N4  | 35:BA:654(M):C:H42  | 2.18                     | 0.41              |
| 35:BA:849:A:C8     | 35:BA:850:C:C5      | 3.07                     | 0.41              |
| 38:BD:28:GLU:O     | 38:BD:29:PRO:C      | 2.57                     | 0.41              |
| 41:BG:137:GLU:O    | 41:BG:138:GLN:O     | 2.37                     | 0.41              |
| 41:BG:42:GLY:O     | 41:BG:43:LEU:CB     | 2.67                     | 0.41              |
| 41:BG:7:LEU:HB2    | 41:BG:104:GLU:CD    | 2.40                     | 0.41              |
| 48:BP:104:GLY:H    | 48:BP:105:LEU:HD12  | 1.85                     | 0.41              |
| 48:BP:114:ILE:CD1  | 48:BP:114:ILE:C     | 2.80                     | 0.41              |
| 48:BP:85:LEU:HA    | 48:BP:88:LEU:CB     | 2.50                     | 0.41              |
| 50:BR:103:ARG:NH1  | 50:BR:110:PRO:HD3   | 2.30                     | 0.41              |
| 51:BS:67:ARG:HH21  | 51:BS:100:ALA:HB3   | 1.85                     | 0.41              |
| 51:BS:68:GLN:O     | 51:BS:70:GLY:N      | 2.52                     | 0.41              |
| 52:BT:96:ARG:HG2   | 52:BT:98:LYS:O      | 2.19                     | 0.41              |
| 53:BU:112:ARG:NH1  | 54:BV:46:VAL:HG11   | 2.35                     | 0.41              |
| 53:BU:49:HIS:C     | 53:BU:51:LYS:N      | 2.70                     | 0.41              |
| 54:BV:15:GLU:HG2   | 54:BV:16:PRO:CD     | 2.50                     | 0.41              |
| 54:BV:16:PRO:HD3   | 54:BV:99:ILE:HD11   | 2.01                     | 0.41              |
| 54:BV:34:GLU:O     | 54:BV:36:PRO:HD3    | 2.20                     | 0.41              |
| 54:BV:35:LEU:HB3   | 54:BV:37:VAL:HG23   | 2.02                     | 0.41              |
| 57:BY:28:LYS:CG    | 57:BY:37:VAL:HB     | 2.49                     | 0.41              |
| 1:AA:116:A:N7      | 1:AA:116:A:OP2      | 2.53                     | 0.41              |
| 1:AA:1222:G:O2'    | 1:AA:1223:C:H5'     | 2.20                     | 0.41              |
| 1:AA:264:U:H6      | 1:AA:264:U:O5'      | 2.03                     | 0.41              |
| 1:AA:304:U:O2'     | 1:AA:305:G:H5'      | 2.19                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:411:A:O2'     | 1:AA:413:G:H5'    | 2.20                     | 0.41              |
| 1:AA:432:A:C8      | 1:AA:433:C:C5     | 3.08                     | 0.41              |
| 1:AA:771:G:C4      | 1:AA:772:U:C5     | 3.07                     | 0.41              |
| 1:AA:773:G:C4      | 1:AA:774:G:N7     | 2.88                     | 0.41              |
| 1:AA:872:A:O3'     | 1:AA:873:A:H2'    | 2.20                     | 0.41              |
| 1:AA:895:G:H2'     | 1:AA:896:C:C6     | 2.54                     | 0.41              |
| 1:AA:973:G:N3      | 10:AJ:55:LYS:CE   | 2.83                     | 0.41              |
| 11:AK:126:ARG:CZ   | 11:AK:126:ARG:HB3 | 2.49                     | 0.41              |
| 16:AP:59:TRP:HA    | 16:AP:62:VAL:HG23 | 2.02                     | 0.41              |
| 16:AP:60:LEU:HA    | 16:AP:60:LEU:HD23 | 1.86                     | 0.41              |
| 24:AY:137:ASN:CG   | 24:AY:138:LYS:N   | 2.73                     | 0.41              |
| 24:AY:343:ASN:ND2  | 24:AY:346:LYS:N   | 2.68                     | 0.41              |
| 24:AY:356:LEU:HD21 | 24:AY:358:MET:SD  | 2.60                     | 0.41              |
| 24:AY:58:GLU:HG3   | 24:AY:65:ILE:HG12 | 2.03                     | 0.41              |
| 25:B0:37:LEU:CD2   | 25:B0:37:LEU:H    | 2.26                     | 0.41              |
| 25:B0:43:THR:O     | 25:B0:44:ARG:C    | 2.58                     | 0.41              |
| 26:B1:86:SER:O     | 26:B1:86:SER:OG   | 2.32                     | 0.41              |
| 30:B5:49:CYS:HB2   | 30:B5:50:GLY:H    | 1.63                     | 0.41              |
| 32:B7:4:THR:HG22   | 35:BA:687:C:O4'   | 2.20                     | 0.41              |
| 33:B8:12:LYS:HG2   | 48:BP:68:GLN:CG   | 2.50                     | 0.41              |
| 35:BA:1475:G:H2'   | 35:BA:1476:C:C6   | 2.55                     | 0.41              |
| 35:BA:1853:A:H2'   | 35:BA:1854:A:C8   | 2.54                     | 0.41              |
| 35:BA:196:A:H5''   | 48:BP:46:LYS:HE2  | 2.01                     | 0.41              |
| 35:BA:2040:C:H2'   | 35:BA:2041:U:H6   | 1.85                     | 0.41              |
| 35:BA:231:C:O2'    | 35:BA:232:G:H5'   | 2.20                     | 0.41              |
| 35:BA:2648:C:H2'   | 35:BA:2649:U:H6   | 1.83                     | 0.41              |
| 35:BA:330:A:HO2'   | 35:BA:331:A:H8    | 1.67                     | 0.41              |
| 35:BA:435:C:C2'    | 35:BA:436:C:H5'   | 2.51                     | 0.41              |
| 35:BA:944:G:H5'    | 35:BA:945:A:C5'   | 2.50                     | 0.41              |
| 35:BA:996:A:H4'    | 53:BU:92:ARG:CD   | 2.51                     | 0.41              |
| 35:BA:1789:A:OP1   | 38:BD:222:ARG:HD3 | 2.20                     | 0.41              |
| 38:BD:48:ARG:NH1   | 38:BD:48:ARG:HG3  | 2.35                     | 0.41              |
| 42:BH:6:ARG:HH11   | 42:BH:6:ARG:CG    | 2.33                     | 0.41              |
| 46:BN:55:VAL:HG22  | 46:BN:126:PRO:HA  | 2.02                     | 0.41              |
| 46:BN:56:ASN:O     | 46:BN:57:ALA:O    | 2.37                     | 0.41              |
| 47:BO:64:ARG:HG2   | 47:BO:79:PHE:CG   | 2.56                     | 0.41              |
| 48:BP:30:THR:CG2   | 48:BP:31:ALA:H    | 2.33                     | 0.41              |
| 48:BP:97:PRO:HG3   | 48:BP:112:LEU:CD1 | 2.50                     | 0.41              |
| 56:BX:27:THR:HB    | 56:BX:80:ILE:HB   | 2.03                     | 0.41              |
| 57:BY:6:HIS:CD2    | 57:BY:6:HIS:H     | 2.38                     | 0.41              |
| 58:BZ:129:SER:O    | 58:BZ:130:PRO:C   | 2.58                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1148:U:H2'   | 1:AA:1149:C:O4'   | 2.19                     | 0.41              |
| 1:AA:204:U:H4'    | 1:AA:216:G:C5'    | 2.48                     | 0.41              |
| 1:AA:668:G:O2'    | 15:AO:46:HIS:CD2  | 2.74                     | 0.41              |
| 2:AB:160:ASP:O    | 2:AB:161:ALA:HB2  | 2.20                     | 0.41              |
| 4:AD:28:SER:OG    | 4:AD:30:LYS:HG2   | 2.21                     | 0.41              |
| 6:AF:42:GLU:HG3   | 6:AF:61:LEU:HD23  | 2.01                     | 0.41              |
| 6:AF:42:GLU:HG3   | 6:AF:61:LEU:CD2   | 2.51                     | 0.41              |
| 9:AI:56:LEU:HB3   | 9:AI:57:GLY:H     | 1.71                     | 0.41              |
| 1:AA:1049:U:O2'   | 14:AN:2:ALA:N     | 2.53                     | 0.41              |
| 16:AP:28:ARG:NH1  | 16:AP:29:ASP:OD2  | 2.54                     | 0.41              |
| 16:AP:21:VAL:HG12 | 16:AP:34:GLU:O    | 2.20                     | 0.41              |
| 18:AR:40:LEU:HB3  | 18:AR:79:LEU:HD11 | 2.02                     | 0.41              |
| 19:AS:47:HIS:O    | 19:AS:62:ILE:CG2  | 2.68                     | 0.41              |
| 20:AT:14:LYS:HE3  | 20:AT:18:GLN:HE22 | 1.85                     | 0.41              |
| 22:AV:12:U:H3     | 22:AV:23:A:H62    | 1.67                     | 0.41              |
| 24:AY:150:ILE:O   | 24:AY:151:ARG:C   | 2.59                     | 0.41              |
| 24:AY:507:TYR:CD1 | 24:AY:508:GLY:N   | 2.88                     | 0.41              |
| 24:AY:95:GLU:OE1  | 24:AY:128:TYR:OH  | 2.37                     | 0.41              |
| 25:B0:67:VAL:HG12 | 25:B0:68:GLU:H    | 1.84                     | 0.41              |
| 26:B1:40:ARG:NH1  | 26:B1:40:ARG:HG2  | 2.35                     | 0.41              |
| 31:B6:8:LYS:HA    | 31:B6:27:LYS:HA   | 2.02                     | 0.41              |
| 33:B8:26:LYS:HB3  | 33:B8:44:LYS:HG3  | 2.01                     | 0.41              |
| 33:B8:4:MET:HE2   | 33:B8:61:LEU:HD23 | 2.03                     | 0.41              |
| 33:B8:62:LEU:O    | 33:B8:64:TYR:N    | 2.53                     | 0.41              |
| 35:BA:1039:G:O6   | 35:BA:1116:C:N3   | 2.53                     | 0.41              |
| 35:BA:1144:G:C4   | 35:BA:1145:C:C5   | 3.08                     | 0.41              |
| 35:BA:1289:C:H2'  | 35:BA:1290:C:C6   | 2.55                     | 0.41              |
| 35:BA:1301:A:H2'  | 35:BA:1302:A:C2'  | 2.51                     | 0.41              |
| 35:BA:1344:G:H4'  | 35:BA:1384:A:C5   | 2.56                     | 0.41              |
| 35:BA:1374:G:O2'  | 35:BA:1375:C:H5'  | 2.19                     | 0.41              |
| 35:BA:1486:A:O4'  | 35:BA:1505:C:N4   | 2.53                     | 0.41              |
| 35:BA:2117:A:O2'  | 35:BA:2118:U:O5'  | 2.35                     | 0.41              |
| 35:BA:2362:G:H2'  | 35:BA:2363:C:C5'  | 2.49                     | 0.41              |
| 35:BA:2611:U:H2'  | 35:BA:2611:U:O2   | 2.20                     | 0.41              |
| 35:BA:2637:U:O2'  | 35:BA:2638:G:H5'  | 2.20                     | 0.41              |
| 35:BA:29:U:H2'    | 35:BA:30:G:C8     | 2.55                     | 0.41              |
| 35:BA:630:G:C4'   | 35:BA:640:C:H4'   | 2.50                     | 0.41              |
| 35:BA:643:A:C2'   | 35:BA:644:A:H5'   | 2.51                     | 0.41              |
| 35:BA:673:C:H5"   | 40:BF:80:ALA:HB1  | 2.02                     | 0.41              |
| 35:BA:664:C:H4'   | 35:BA:941:A:OP1   | 2.20                     | 0.41              |
| 28:B3:13:ILE:HD11 | 35:BA:989:G:C8    | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BB:77:U:P       | 58:BZ:19:ARG:HH22  | 2.43                     | 0.41              |
| 36:BB:91:C:OP1     | 49:BQ:16:ARG:HG3   | 2.20                     | 0.41              |
| 38:BD:102:LYS:C    | 38:BD:103:ARG:HG2  | 2.40                     | 0.41              |
| 38:BD:129:ASN:O    | 38:BD:193:VAL:HG12 | 2.20                     | 0.41              |
| 38:BD:65:ILE:O     | 38:BD:65:ILE:HD13  | 2.21                     | 0.41              |
| 39:BE:47:VAL:HG22  | 39:BE:84:PHE:O     | 2.20                     | 0.41              |
| 41:BG:60:LEU:HA    | 41:BG:63:ILE:HG23  | 2.02                     | 0.41              |
| 46:BN:45:ASN:ND2   | 46:BN:45:ASN:N     | 2.67                     | 0.41              |
| 52:BT:85:LYS:NZ    | 52:BT:85:LYS:CB    | 2.54                     | 0.41              |
| 53:BU:66:ASN:HD21  | 53:BU:70:ARG:HE    | 1.67                     | 0.41              |
| 57:BY:49:VAL:O     | 57:BY:50:ARG:CB    | 2.67                     | 0.41              |
| 57:BY:95:LYS:HD2   | 57:BY:99:CYS:O     | 2.20                     | 0.41              |
| 58:BZ:155:LEU:CD2  | 58:BZ:155:LEU:N    | 2.83                     | 0.41              |
| 58:BZ:60:GLU:O     | 58:BZ:61:LEU:HB2   | 2.20                     | 0.41              |
| 1:AA:1070:U:O2'    | 1:AA:1071:C:H5'    | 2.21                     | 0.41              |
| 1:AA:1152:A:C2'    | 1:AA:1153:C:O5'    | 2.69                     | 0.41              |
| 1:AA:1118:C:O2     | 1:AA:1179:A:C6     | 2.74                     | 0.41              |
| 1:AA:149:A:H2'     | 1:AA:150:C:C6      | 2.55                     | 0.41              |
| 1:AA:266:G:O2'     | 1:AA:267:C:OP2     | 2.35                     | 0.41              |
| 1:AA:431:A:H2'     | 1:AA:432:A:O4'     | 2.20                     | 0.41              |
| 1:AA:701:C:H1'     | 1:AA:703:G:C2      | 2.55                     | 0.41              |
| 1:AA:917:G:C2'     | 1:AA:918:A:H5'     | 2.50                     | 0.41              |
| 2:AB:114:ARG:NH1   | 2:AB:141:GLU:OE2   | 2.54                     | 0.41              |
| 2:AB:19:HIS:HE2    | 2:AB:206:ASP:CG    | 2.23                     | 0.41              |
| 3:AC:151:VAL:O     | 3:AC:167:TRP:HA    | 2.20                     | 0.41              |
| 4:AD:31:CYS:O      | 4:AD:32:ALA:HB3    | 2.20                     | 0.41              |
| 5:AE:50:GLU:CD     | 5:AE:51:VAL:H      | 2.24                     | 0.41              |
| 7:AG:152:ALA:HB1   | 7:AG:155:ARG:NH2   | 2.36                     | 0.41              |
| 2:AB:181:PHE:HD1   | 8:AH:70:GLN:HB3    | 1.86                     | 0.41              |
| 9:AI:85:LEU:C      | 9:AI:85:LEU:HD12   | 2.41                     | 0.41              |
| 20:AT:14:LYS:HA    | 20:AT:17:ARG:NE    | 2.36                     | 0.41              |
| 24:AY:435:ASP:OD1  | 24:AY:437:THR:HB   | 2.20                     | 0.41              |
| 24:AY:517:LEU:HD13 | 24:AY:563:ILE:HA   | 2.01                     | 0.41              |
| 25:B0:19:LYS:NZ    | 25:B0:19:LYS:HB3   | 2.23                     | 0.41              |
| 33:B8:48:PHE:HB3   | 33:B8:49:VAL:H     | 1.75                     | 0.41              |
| 35:BA:1290:C:O5'   | 35:BA:1290:C:H6    | 2.04                     | 0.41              |
| 35:BA:1381:G:O2'   | 35:BA:1382:G:C5'   | 2.68                     | 0.41              |
| 35:BA:1495:A:N3    | 35:BA:1495:A:H2'   | 2.35                     | 0.41              |
| 35:BA:1528:A:N1    | 35:BA:1542:A:C2    | 2.88                     | 0.41              |
| 35:BA:156:U:C2'    | 35:BA:157:U:H5'    | 2.50                     | 0.41              |
| 35:BA:157:U:C2'    | 35:BA:158:U:H5'    | 2.50                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:1692:U:O2'   | 35:BA:1693:U:H2'  | 2.20                     | 0.41              |
| 35:BA:1805:U:C2'   | 35:BA:1806:C:C5'  | 2.88                     | 0.41              |
| 35:BA:1996:C:OP1   | 35:BA:1996:C:H6   | 2.03                     | 0.41              |
| 35:BA:20:C:O2'     | 35:BA:21:A:H5'    | 2.20                     | 0.41              |
| 35:BA:262:A:HO2'   | 35:BA:263:C:H5'   | 1.79                     | 0.41              |
| 35:BA:2680:C:OP2   | 39:BE:111:ARG:NH2 | 2.51                     | 0.41              |
| 35:BA:385:C:O2'    | 35:BA:388:G:N2    | 2.53                     | 0.41              |
| 35:BA:942:G:C2'    | 35:BA:943:U:H5'   | 2.50                     | 0.41              |
| 35:BA:955:C:O2'    | 35:BA:956:G:C5'   | 2.57                     | 0.41              |
| 36:BB:43:C:H1'     | 41:BG:94:LEU:HD22 | 2.02                     | 0.41              |
| 35:BA:773:U:H4'    | 38:BD:47:GLY:HA3  | 2.01                     | 0.41              |
| 39:BE:77:ILE:CG2   | 39:BE:78:LEU:HD12 | 2.51                     | 0.41              |
| 43:BJ:44:UNK:O     | 43:BJ:48:UNK:CB   | 2.68                     | 0.41              |
| 43:BJ:94:UNK:C     | 43:BJ:96:UNK:N    | 2.82                     | 0.41              |
| 44:BK:89:UNK:C     | 44:BK:91:UNK:N    | 2.82                     | 0.41              |
| 49:BQ:66:ILE:HG13  | 49:BQ:66:ILE:H    | 1.66                     | 0.41              |
| 51:BS:83:LYS:HG2   | 51:BS:83:LYS:O    | 2.20                     | 0.41              |
| 54:BV:5:VAL:CG2    | 54:BV:35:LEU:HB3  | 2.50                     | 0.41              |
| 57:BY:31:LEU:HD13  | 57:BY:31:LEU:HA   | 1.92                     | 0.41              |
| 58:BZ:119:GLU:HG2  | 58:BZ:119:GLU:O   | 2.20                     | 0.41              |
| 58:BZ:12:GLY:HA2   | 58:BZ:36:LYS:NZ   | 2.35                     | 0.41              |
| 1:AA:1048:G:C6     | 1:AA:1210:C:N4    | 2.89                     | 0.41              |
| 1:AA:1442(A):G:H2' | 52:BT:122:ASP:OD2 | 2.21                     | 0.41              |
| 1:AA:494:U:O5'     | 1:AA:494:U:C6     | 2.59                     | 0.41              |
| 1:AA:671:G:H2'     | 1:AA:672:U:O4'    | 2.20                     | 0.41              |
| 1:AA:683:G:H3'     | 1:AA:684:A:C8     | 2.56                     | 0.41              |
| 1:AA:696:A:H1'     | 1:AA:786:G:O2'    | 2.21                     | 0.41              |
| 1:AA:711:G:O2'     | 1:AA:712:A:H5'    | 2.20                     | 0.41              |
| 1:AA:939:G:H1      | 1:AA:1344:C:N4    | 2.13                     | 0.41              |
| 1:AA:946:A:N6      | 1:AA:947:G:O6     | 2.54                     | 0.41              |
| 1:AA:957:U:H4'     | 19:AS:79:THR:O    | 2.21                     | 0.41              |
| 2:AB:10:LEU:C      | 2:AB:10:LEU:CD2   | 2.88                     | 0.41              |
| 2:AB:130:ARG:O     | 2:AB:131:PRO:C    | 2.59                     | 0.41              |
| 2:AB:87:ARG:HD3    | 2:AB:219:VAL:CG1  | 2.49                     | 0.41              |
| 2:AB:32:ILE:HD13   | 2:AB:40:HIS:CD2   | 2.55                     | 0.41              |
| 3:AC:122:GLU:C     | 3:AC:124:ILE:N    | 2.74                     | 0.41              |
| 3:AC:123:GLN:HE21  | 3:AC:123:GLN:HA   | 1.86                     | 0.41              |
| 3:AC:29:TYR:O      | 3:AC:30:ARG:C     | 2.59                     | 0.41              |
| 4:AD:3:ARG:H       | 4:AD:3:ARG:CD     | 2.25                     | 0.41              |
| 5:AE:139:LEU:HD23  | 5:AE:142:LEU:HD11 | 2.02                     | 0.41              |
| 8:AH:1:MET:O       | 8:AH:2:LEU:CB     | 2.69                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 9:AI:49:PRO:HG2     | 9:AI:81:ILE:CG2    | 2.43                     | 0.41              |
| 9:AI:59:PHE:CZ      | 9:AI:88:TYR:CE2    | 3.07                     | 0.41              |
| 12:AL:7:ILE:O       | 12:AL:11:VAL:HG23  | 2.20                     | 0.41              |
| 16:AP:21:VAL:CG1    | 16:AP:34:GLU:HB3   | 2.50                     | 0.41              |
| 24:AY:266:ASN:C     | 24:AY:267:LYS:HG3  | 2.41                     | 0.41              |
| 24:AY:635:GLU:OE2   | 24:AY:644:ARG:NH1  | 2.54                     | 0.41              |
| 26:B1:82:LEU:HA     | 26:B1:82:LEU:HD12  | 1.82                     | 0.41              |
| 28:B3:7:LYS:CB      | 28:B3:34:GLU:HB3   | 2.49                     | 0.41              |
| 29:B4:28:LYS:NZ     | 41:BG:144:ILE:HG22 | 2.36                     | 0.41              |
| 29:B4:53:GLU:OE1    | 29:B4:54:GLY:N     | 2.54                     | 0.41              |
| 31:B6:6:ARG:CB      | 31:B6:6:ARG:NH1    | 2.78                     | 0.41              |
| 35:BA:1318:C:C3'    | 35:BA:1319:G:H5''  | 2.47                     | 0.41              |
| 35:BA:1505:C:O4'    | 35:BA:1505:C:O2    | 2.39                     | 0.41              |
| 35:BA:1509(B):A:H2' | 35:BA:1510:G:C8    | 2.55                     | 0.41              |
| 35:BA:749:C:O2      | 35:BA:1618:A:H2'   | 2.20                     | 0.41              |
| 35:BA:1636:C:H2'    | 35:BA:1637:A:C8    | 2.55                     | 0.41              |
| 35:BA:1748:G:H2'    | 35:BA:1749:A:O4'   | 2.20                     | 0.41              |
| 35:BA:1887:C:H2'    | 35:BA:1888:G:C4'   | 2.51                     | 0.41              |
| 35:BA:1855:G:N2     | 35:BA:1888:G:H1'   | 2.36                     | 0.41              |
| 35:BA:1893:C:H2'    | 35:BA:1894:C:O4'   | 2.20                     | 0.41              |
| 35:BA:2006:C:N4     | 35:BA:2007:C:N4    | 2.68                     | 0.41              |
| 35:BA:2176:A:O2'    | 35:BA:2177:C:P     | 2.79                     | 0.41              |
| 35:BA:2523:G:H2'    | 35:BA:2524:G:H5'   | 2.01                     | 0.41              |
| 35:BA:2528:U:H2'    | 35:BA:2530:A:O5'   | 2.20                     | 0.41              |
| 35:BA:245:G:C6      | 35:BA:254:G:N2     | 2.88                     | 0.41              |
| 35:BA:2666:C:H5'    | 35:BA:2667:C:OP2   | 2.20                     | 0.41              |
| 35:BA:361:G:H2'     | 35:BA:362:U:C5'    | 2.42                     | 0.41              |
| 35:BA:483:A:H2'     | 35:BA:484:C:O4'    | 2.20                     | 0.41              |
| 35:BA:569:U:C4      | 35:BA:570:G:C6     | 3.08                     | 0.41              |
| 35:BA:747:U:O4      | 35:BA:2613:U:C2    | 2.72                     | 0.41              |
| 35:BA:962:G:H2'     | 35:BA:963:U:C5'    | 2.47                     | 0.41              |
| 36:BB:7:G:C3'       | 36:BB:8:U:C5'      | 2.99                     | 0.41              |
| 37:BC:11:LEU:HD22   | 37:BC:11:LEU:H     | 1.86                     | 0.41              |
| 37:BC:149:ASN:O     | 37:BC:151:GLY:N    | 2.54                     | 0.41              |
| 38:BD:142:VAL:HG22  | 38:BD:143:HIS:N    | 2.36                     | 0.41              |
| 38:BD:165:ILE:HA    | 38:BD:175:LEU:HD23 | 2.03                     | 0.41              |
| 38:BD:68:LYS:HD3    | 38:BD:70:TRP:CZ2   | 2.55                     | 0.41              |
| 40:BF:102:PRO:HB2   | 40:BF:105:VAL:CG2  | 2.49                     | 0.41              |
| 41:BG:135:LEU:HD12  | 41:BG:135:LEU:H    | 1.84                     | 0.41              |
| 42:BH:11:VAL:HG13   | 42:BH:12:PRO:HD2   | 2.03                     | 0.41              |
| 46:BN:37:LYS:HG3    | 46:BN:42:TRP:CZ3   | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:BO:87:ILE:HD13  | 47:BO:93:PRO:HA    | 2.02                     | 0.41              |
| 48:BP:47:ASP:OD2   | 48:BP:49:ARG:CA    | 2.69                     | 0.41              |
| 49:BQ:32:TYR:O     | 49:BQ:105:GLU:CB   | 2.66                     | 0.41              |
| 49:BQ:48:GLU:O     | 49:BQ:52:VAL:HG23  | 2.20                     | 0.41              |
| 51:BS:101:LEU:C    | 51:BS:101:LEU:HD12 | 2.41                     | 0.41              |
| 52:BT:35:LYS:NZ    | 52:BT:41:ARG:CD    | 2.83                     | 0.41              |
| 53:BU:112:ARG:NH2  | 54:BV:46:VAL:HG13  | 2.35                     | 0.41              |
| 1:AA:1030(A):G:C6  | 1:AA:1030(B):C:N4  | 2.89                     | 0.41              |
| 1:AA:66:G:C6       | 1:AA:104:G:C2      | 3.09                     | 0.41              |
| 1:AA:1505:G:C8     | 1:AA:1505:G:OP2    | 2.73                     | 0.41              |
| 1:AA:1508:G:H2'    | 1:AA:1509:C:C6     | 2.56                     | 0.41              |
| 1:AA:1527:C:O5'    | 1:AA:1527:C:H6     | 2.03                     | 0.41              |
| 1:AA:409:G:OP1     | 4:AD:22:LYS:O      | 2.38                     | 0.41              |
| 1:AA:490:G:H2'     | 1:AA:491:G:O5'     | 2.20                     | 0.41              |
| 1:AA:498:U:HO2'    | 1:AA:499:A:P       | 2.43                     | 0.41              |
| 1:AA:538:G:H2'     | 1:AA:539:A:C8      | 2.56                     | 0.41              |
| 1:AA:862:C:C3'     | 1:AA:863:U:C5'     | 2.98                     | 0.41              |
| 1:AA:878:G:C5'     | 8:AH:89:PRO:HG2    | 2.51                     | 0.41              |
| 1:AA:958:A:C6      | 1:AA:959:A:N1      | 2.89                     | 0.41              |
| 1:AA:999:C:O2'     | 1:AA:1000:U:H5'    | 2.20                     | 0.41              |
| 2:AB:42:ILE:CD1    | 2:AB:202:PRO:C     | 2.89                     | 0.41              |
| 2:AB:9:GLU:CD      | 2:AB:9:GLU:N       | 2.74                     | 0.41              |
| 3:AC:191:THR:HG21  | 3:AC:193:TYR:CE1   | 2.55                     | 0.41              |
| 3:AC:69:HIS:HA     | 3:AC:104:GLN:HB2   | 2.02                     | 0.41              |
| 8:AH:72:PRO:O      | 8:AH:73:ASP:CB     | 2.69                     | 0.41              |
| 9:AI:17:VAL:HG11   | 9:AI:80:GLY:C      | 2.41                     | 0.41              |
| 10:AJ:47:PHE:CE2   | 14:AN:37:PHE:HE2   | 2.38                     | 0.41              |
| 10:AJ:78:ASN:ND2   | 10:AJ:80:LYS:H     | 2.06                     | 0.41              |
| 12:AL:18:VAL:O     | 12:AL:19:ARG:CB    | 2.68                     | 0.41              |
| 17:AQ:74:LEU:HD13  | 17:AQ:74:LEU:C     | 2.41                     | 0.41              |
| 24:AY:137:ASN:HD22 | 24:AY:138:LYS:H    | 1.59                     | 0.41              |
| 24:AY:150:ILE:CD1  | 24:AY:163:VAL:HG22 | 2.51                     | 0.41              |
| 24:AY:31:ARG:HD2   | 24:AY:263:ALA:O    | 2.20                     | 0.41              |
| 26:B1:26:ARG:O     | 26:B1:27:GLU:C     | 2.59                     | 0.41              |
| 29:B4:61:ARG:N     | 29:B4:61:ARG:NH1   | 2.69                     | 0.41              |
| 31:B6:44:ARG:HA    | 31:B6:44:ARG:HD2   | 1.85                     | 0.41              |
| 27:B2:7:ARG:NH2    | 35:BA:102:G:OP2    | 2.53                     | 0.41              |
| 35:BA:1111:A:O4'   | 42:BH:1:MET:SD     | 2.79                     | 0.41              |
| 35:BA:1386:C:H2'   | 35:BA:1387:C:C6    | 2.56                     | 0.41              |
| 35:BA:1599:C:HO2'  | 35:BA:1600:C:H5'   | 1.84                     | 0.41              |
| 35:BA:1750:G:O2'   | 35:BA:1751:C:H5'   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:1770:G:C6    | 35:BA:1771:C:C4   | 3.08                     | 0.41              |
| 35:BA:1790:C:H5''  | 35:BA:1791:A:OP1  | 2.20                     | 0.41              |
| 35:BA:2153:G:H2'   | 35:BA:2153:G:N3   | 2.34                     | 0.41              |
| 35:BA:2320:A:N3    | 35:BA:2320:A:H2'  | 2.36                     | 0.41              |
| 35:BA:2402:C:C1'   | 35:BA:2403:C:OP2  | 2.69                     | 0.41              |
| 35:BA:2553:G:H8    | 35:BA:2553:G:O5'  | 2.04                     | 0.41              |
| 35:BA:2577:A:H5''  | 35:BA:2578:G:H5'  | 2.02                     | 0.41              |
| 35:BA:257:A:H2'    | 35:BA:258:G:H8    | 1.86                     | 0.41              |
| 35:BA:2606:C:C2    | 35:BA:2607:G:C8   | 3.08                     | 0.41              |
| 35:BA:2836:U:O5'   | 35:BA:2836:U:H6   | 2.02                     | 0.41              |
| 35:BA:600:G:H2'    | 35:BA:601:C:C6    | 2.54                     | 0.41              |
| 30:B5:2:ALA:N      | 35:BA:747:U:C4    | 2.89                     | 0.41              |
| 36:BB:35:U:O2'     | 36:BB:36:C:H5'    | 2.21                     | 0.41              |
| 36:BB:22:U:H3      | 36:BB:61:G:H1     | 1.68                     | 0.41              |
| 39:BE:103:ASP:CG   | 39:BE:201:THR:HA  | 2.41                     | 0.41              |
| 40:BF:19:GLU:HA    | 40:BF:24:LEU:HD21 | 2.02                     | 0.41              |
| 40:BF:78:ILE:HG13  | 40:BF:78:ILE:O    | 2.20                     | 0.41              |
| 42:BH:105:LEU:HD23 | 42:BH:105:LEU:H   | 1.84                     | 0.41              |
| 42:BH:5:GLY:HA2    | 42:BH:69:ARG:CB   | 2.50                     | 0.41              |
| 42:BH:70:THR:O     | 42:BH:74:ASN:ND2  | 2.52                     | 0.41              |
| 42:BH:92:ILE:C     | 42:BH:94:TYR:H    | 2.23                     | 0.41              |
| 44:BK:107:UNK:O    | 44:BK:108:UNK:C   | 2.68                     | 0.41              |
| 45:BL:81:UNK:C     | 45:BL:83:UNK:N    | 2.84                     | 0.41              |
| 49:BQ:75:THR:HG23  | 49:BQ:76:LYS:N    | 2.34                     | 0.41              |
| 50:BR:10:LEU:HB2   | 50:BR:11:ASN:H    | 1.52                     | 0.41              |
| 52:BT:16:ARG:CG    | 52:BT:16:ARG:HH11 | 2.34                     | 0.41              |
| 52:BT:34:VAL:HA    | 52:BT:39:ARG:HA   | 2.03                     | 0.41              |
| 53:BU:112:ARG:NH1  | 54:BV:46:VAL:CG1  | 2.83                     | 0.41              |
| 35:BA:2011:U:OP2   | 55:BW:16:LYS:HD3  | 2.21                     | 0.41              |
| 57:BY:45:VAL:HG11  | 57:BY:60:PHE:HB3  | 2.02                     | 0.41              |
| 58:BZ:20:ARG:CB    | 58:BZ:20:ARG:NH1  | 2.84                     | 0.41              |
| 58:BZ:96:VAL:O     | 58:BZ:127:LYS:HA  | 2.20                     | 0.41              |
| 1:AA:1385:G:H2'    | 1:AA:1386:G:O5'   | 2.21                     | 0.41              |
| 1:AA:198:G:O2'     | 1:AA:199:G:OP2    | 2.38                     | 0.41              |
| 1:AA:269:C:H2'     | 1:AA:270:A:H8     | 1.86                     | 0.41              |
| 1:AA:323:U:O5'     | 1:AA:323:U:H6     | 2.03                     | 0.41              |
| 1:AA:530:G:H3'     | 1:AA:531:U:H5'    | 2.01                     | 0.41              |
| 1:AA:592:G:N3      | 1:AA:593:G:C8     | 2.89                     | 0.41              |
| 1:AA:892:A:C2      | 1:AA:907:A:C4     | 3.09                     | 0.41              |
| 1:AA:960:U:O2'     | 1:AA:1223:C:C5'   | 2.68                     | 0.41              |
| 7:AG:22:LEU:C      | 7:AG:24:THR:N     | 2.74                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:24:THR:O      | 7:AG:25:ALA:C      | 2.59                     | 0.41              |
| 10:AJ:76:ASN:HA    | 10:AJ:77:PRO:HD2   | 1.96                     | 0.41              |
| 11:AK:21:ILE:CD1   | 11:AK:21:ILE:N     | 2.83                     | 0.41              |
| 13:AM:29:ARG:O     | 13:AM:30:ALA:C     | 2.59                     | 0.41              |
| 19:AS:60:VAL:HG13  | 19:AS:60:VAL:O     | 2.20                     | 0.41              |
| 24:AY:438:PHE:CE1  | 24:AY:451:ILE:CG1  | 3.04                     | 0.41              |
| 24:AY:459:LEU:CD1  | 24:AY:459:LEU:H    | 2.32                     | 0.41              |
| 24:AY:546:ILE:HG12 | 24:AY:590:ILE:HG12 | 2.02                     | 0.41              |
| 25:B0:24:LYS:HA    | 25:B0:24:LYS:HD3   | 1.89                     | 0.41              |
| 25:B0:7:LEU:HB3    | 49:BQ:85:LYS:CG    | 2.46                     | 0.41              |
| 29:B4:55:ARG:O     | 29:B4:56:VAL:C     | 2.57                     | 0.41              |
| 33:B8:62:LEU:C     | 33:B8:64:TYR:N     | 2.74                     | 0.41              |
| 35:BA:1144:G:H2'   | 35:BA:1145:C:H6    | 1.84                     | 0.41              |
| 35:BA:1817:G:OP1   | 38:BD:88:ARG:NH2   | 2.50                     | 0.41              |
| 35:BA:2131:G:C5'   | 35:BA:2133:A:O4'   | 2.69                     | 0.41              |
| 35:BA:2355:C:C4    | 35:BA:2356:C:C4    | 3.08                     | 0.41              |
| 35:BA:247:G:H1'    | 35:BA:251:A:H62    | 1.86                     | 0.41              |
| 35:BA:2612:C:C2'   | 35:BA:2613:U:H5'   | 2.51                     | 0.41              |
| 35:BA:27:G:O2'     | 35:BA:28:A:OP2     | 2.30                     | 0.41              |
| 35:BA:380:U:O2'    | 35:BA:381:G:H5'    | 2.20                     | 0.41              |
| 35:BA:600:G:C2'    | 35:BA:601:C:C5'    | 2.98                     | 0.41              |
| 35:BA:732:C:H2'    | 35:BA:733:G:O4'    | 2.21                     | 0.41              |
| 38:BD:266:SER:C    | 38:BD:267:SER:O    | 2.59                     | 0.41              |
| 39:BE:203:LYS:C    | 39:BE:203:LYS:CD   | 2.88                     | 0.41              |
| 39:BE:68:ALA:O     | 39:BE:70:ALA:N     | 2.54                     | 0.41              |
| 40:BF:8:GLN:O      | 40:BF:10:PRO:N     | 2.53                     | 0.41              |
| 40:BF:8:GLN:CB     | 40:BF:126:VAL:HA   | 2.44                     | 0.41              |
| 40:BF:126:VAL:HG22 | 40:BF:195:ASP:HA   | 2.02                     | 0.41              |
| 40:BF:185:ASP:HA   | 40:BF:188:ARG:CD   | 2.50                     | 0.41              |
| 40:BF:19:GLU:CA    | 40:BF:24:LEU:HD21  | 2.51                     | 0.41              |
| 41:BG:56:ALA:HB2   | 41:BG:153:ARG:NH1  | 2.36                     | 0.41              |
| 41:BG:67:LYS:HG2   | 41:BG:68:PRO:O     | 2.20                     | 0.41              |
| 42:BH:107:VAL:O    | 42:BH:152:ARG:NE   | 2.51                     | 0.41              |
| 46:BN:73:THR:CG2   | 46:BN:82:LEU:HD11  | 2.50                     | 0.41              |
| 48:BP:111:ARG:HA   | 48:BP:128:HIS:CD2  | 2.56                     | 0.41              |
| 48:BP:70:GLN:HB3   | 48:BP:72:PRO:HD2   | 2.02                     | 0.41              |
| 49:BQ:133:ARG:O    | 49:BQ:137:TYR:HE2  | 2.04                     | 0.41              |
| 49:BQ:29:PHE:HB3   | 49:BQ:65:PHE:CD2   | 2.55                     | 0.41              |
| 51:BS:66:ALA:O     | 51:BS:69:VAL:HG12  | 2.20                     | 0.41              |
| 47:BO:104:ARG:NH2  | 52:BT:33:LYS:HE3   | 2.31                     | 0.41              |
| 53:BU:82:GLY:O     | 53:BU:86:ALA:N     | 2.41                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:182:LYS:O    | 58:BZ:183:LEU:HB3  | 2.21                     | 0.41              |
| 1:AA:1003:G:O2'    | 1:AA:1004:A:O5'    | 2.29                     | 0.41              |
| 1:AA:1059:C:O3'    | 14:AN:45:ARG:NH2   | 2.53                     | 0.41              |
| 1:AA:1073:U:H2'    | 1:AA:1074:G:H8     | 1.86                     | 0.41              |
| 1:AA:1149:C:P      | 9:AI:9:ARG:NH1     | 2.94                     | 0.41              |
| 1:AA:1226:C:H4'    | 19:AS:80:TYR:CZ    | 2.55                     | 0.41              |
| 1:AA:175:C:H2'     | 1:AA:176:C:C6      | 2.54                     | 0.41              |
| 1:AA:269:C:H2'     | 1:AA:270:A:C8      | 2.56                     | 0.41              |
| 1:AA:307:C:C5      | 1:AA:308:C:C5      | 3.08                     | 0.41              |
| 1:AA:356:A:C1'     | 1:AA:368:U:O2'     | 2.67                     | 0.41              |
| 1:AA:490:G:C2'     | 1:AA:491:G:O5'     | 2.69                     | 0.41              |
| 1:AA:593:G:H1      | 1:AA:646:U:H3      | 1.68                     | 0.41              |
| 1:AA:872:A:H2'     | 1:AA:872:A:N3      | 2.35                     | 0.41              |
| 2:AB:58:ILE:CG2    | 2:AB:222:ILE:CD1   | 2.99                     | 0.41              |
| 4:AD:31:CYS:C      | 4:AD:33:MET:N      | 2.74                     | 0.41              |
| 7:AG:140:ASP:C     | 7:AG:142:GLU:N     | 2.71                     | 0.41              |
| 11:AK:79:SER:HB2   | 11:AK:106:LYS:HG3  | 2.03                     | 0.41              |
| 12:AL:86:ARG:HB2   | 12:AL:101:VAL:HG23 | 2.03                     | 0.41              |
| 15:AO:39:LEU:HD13  | 15:AO:56:LEU:CD2   | 2.51                     | 0.41              |
| 16:AP:81:ARG:HD3   | 16:AP:83:GLU:OE2   | 2.21                     | 0.41              |
| 1:AA:955:U:H4'     | 19:AS:85:LYS:O     | 2.20                     | 0.41              |
| 24:AY:367:GLU:O    | 24:AY:367:GLU:HG2  | 2.21                     | 0.41              |
| 29:B4:2:LYS:C      | 29:B4:2:LYS:HD3    | 2.41                     | 0.41              |
| 31:B6:8:LYS:HE3    | 31:B6:25:LYS:CD    | 2.51                     | 0.41              |
| 31:B6:27:LYS:O     | 31:B6:28:ARG:C     | 2.59                     | 0.41              |
| 35:BA:1047:G:C2'   | 35:BA:1110:G:H21   | 2.31                     | 0.41              |
| 35:BA:1092:C:H2'   | 35:BA:1093:G:H5'   | 2.02                     | 0.41              |
| 35:BA:115:C:H2'    | 35:BA:116:C:H6     | 1.84                     | 0.41              |
| 35:BA:1360:A:C8    | 35:BA:1361:G:C8    | 3.09                     | 0.41              |
| 35:BA:1472:A:C2'   | 35:BA:1473:G:H5'   | 2.51                     | 0.41              |
| 35:BA:1569:A:O5'   | 38:BD:59:LYS:NZ    | 2.53                     | 0.41              |
| 35:BA:1589:C:H2'   | 35:BA:1590:U:C6    | 2.56                     | 0.41              |
| 35:BA:1994:C:H2'   | 35:BA:1995:U:H5'   | 2.03                     | 0.41              |
| 35:BA:2097:C:H2'   | 35:BA:2098:U:O4'   | 2.21                     | 0.41              |
| 35:BA:2584:U:H2'   | 35:BA:2585:U:H5'   | 2.03                     | 0.41              |
| 35:BA:30:G:H2'     | 35:BA:31:C:H6      | 1.75                     | 0.41              |
| 35:BA:917:A:H2'    | 35:BA:918:A:O4'    | 2.20                     | 0.41              |
| 37:BC:117:THR:HG22 | 37:BC:118:PRO:CA   | 2.42                     | 0.41              |
| 40:BF:110:LEU:O    | 40:BF:114:VAL:HG23 | 2.21                     | 0.41              |
| 40:BF:30:PRO:O     | 40:BF:31:HIS:C     | 2.59                     | 0.41              |
| 40:BF:59:TYR:HE2   | 40:BF:85:GLY:O     | 2.04                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:103:LEU:HD13 | 41:BG:107:LEU:HB2  | 2.03                     | 0.41              |
| 41:BG:77:ILE:HD11  | 41:BG:82:LEU:HD12  | 2.03                     | 0.41              |
| 42:BH:56:SER:HB2   | 42:BH:61:HIS:CE1   | 2.55                     | 0.41              |
| 44:BK:48:UNK:O     | 44:BK:50:UNK:N     | 2.54                     | 0.41              |
| 46:BN:10:GLU:CD    | 46:BN:11:PRO:HD2   | 2.40                     | 0.41              |
| 48:BP:13:ASN:HB3   | 48:BP:14:LYS:H     | 1.49                     | 0.41              |
| 49:BQ:25:ASP:OD2   | 58:BZ:78:LYS:HD3   | 2.20                     | 0.41              |
| 49:BQ:28:ALA:O     | 49:BQ:29:PHE:HD1   | 2.03                     | 0.41              |
| 51:BS:96:GLY:O     | 51:BS:98:VAL:N     | 2.52                     | 0.41              |
| 55:BW:43:GLY:O     | 55:BW:44:ALA:C     | 2.58                     | 0.41              |
| 57:BY:20:TYR:N     | 57:BY:20:TYR:CD1   | 2.89                     | 0.41              |
| 1:AA:1267:C:O2'    | 1:AA:1268:A:O5'    | 2.38                     | 0.41              |
| 1:AA:1372:U:H2'    | 1:AA:1373:G:C8     | 2.54                     | 0.41              |
| 1:AA:1452:C:H5'    | 1:AA:1457:G:C8     | 2.56                     | 0.41              |
| 1:AA:1507:A:C2     | 1:AA:1508:G:C4     | 3.09                     | 0.41              |
| 1:AA:185:A:C5      | 1:AA:186:C:N4      | 2.89                     | 0.41              |
| 1:AA:203:U:H6      | 1:AA:203:U:OP2     | 2.03                     | 0.41              |
| 1:AA:563:A:H2      | 12:AL:15:ARG:NH2   | 2.19                     | 0.41              |
| 2:AB:82:ARG:NH1    | 2:AB:86:GLU:OE2    | 2.53                     | 0.41              |
| 12:AL:27:LEU:HB2   | 12:AL:62:SER:HB2   | 2.03                     | 0.41              |
| 13:AM:116:THR:HG22 | 13:AM:117:VAL:N    | 2.31                     | 0.41              |
| 19:AS:17:GLU:C     | 19:AS:19:VAL:N     | 2.73                     | 0.41              |
| 19:AS:61:TYR:O     | 19:AS:62:ILE:C     | 2.59                     | 0.41              |
| 19:AS:60:VAL:O     | 19:AS:62:ILE:HG22  | 2.21                     | 0.41              |
| 1:AA:1314:C:H5     | 19:AS:6:LYS:NZ     | 2.16                     | 0.41              |
| 24:AY:100:VAL:HG13 | 24:AY:101:LEU:N    | 2.35                     | 0.41              |
| 24:AY:107:VAL:HG12 | 24:AY:108:PHE:N    | 2.35                     | 0.41              |
| 24:AY:181:LEU:HD21 | 24:AY:243:VAL:CG2  | 2.51                     | 0.41              |
| 24:AY:74:TRP:CE2   | 24:AY:273:LEU:HB3  | 2.55                     | 0.41              |
| 24:AY:356:LEU:HD23 | 24:AY:356:LEU:O    | 2.21                     | 0.41              |
| 24:AY:529:ILE:HD11 | 24:AY:534:ILE:HD12 | 2.03                     | 0.41              |
| 25:B0:46:LYS:HA    | 25:B0:47:PRO:HD3   | 1.93                     | 0.41              |
| 28:B3:18:ASP:N     | 28:B3:18:ASP:OD1   | 2.53                     | 0.41              |
| 35:BA:1297:C:O2'   | 35:BA:1298:C:C5'   | 2.44                     | 0.41              |
| 35:BA:1288:U:C2    | 35:BA:1327:C:C2    | 3.09                     | 0.41              |
| 35:BA:1362:C:O2'   | 35:BA:1363:C:H5'   | 2.21                     | 0.41              |
| 35:BA:1510:G:O2'   | 35:BA:1511:C:H5'   | 2.21                     | 0.41              |
| 35:BA:2070:G:H2'   | 35:BA:2071:A:C8    | 2.55                     | 0.41              |
| 35:BA:266:G:H2'    | 35:BA:267:C:O5'    | 2.21                     | 0.41              |
| 35:BA:28:A:C5      | 35:BA:29:U:C5      | 3.09                     | 0.41              |
| 35:BA:332:A:N1     | 35:BA:335:C:C5     | 2.88                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:337:C:H2'   | 35:BA:338:G:O4'    | 2.21                     | 0.41              |
| 35:BA:405:U:O2    | 35:BA:405:U:O4'    | 2.39                     | 0.41              |
| 35:BA:637:A:C2    | 35:BA:652:C:H5'    | 2.56                     | 0.41              |
| 35:BA:964:C:H6    | 35:BA:964:C:O5'    | 2.04                     | 0.41              |
| 37:BC:129:GLY:HA3 | 37:BC:138:LEU:HD12 | 2.02                     | 0.41              |
| 37:BC:11:LEU:CD1  | 37:BC:33:LEU:HA    | 2.50                     | 0.41              |
| 38:BD:231:HIS:CD2 | 38:BD:249:PRO:HB3  | 2.56                     | 0.41              |
| 38:BD:238:GLY:O   | 38:BD:239:ARG:O    | 2.39                     | 0.41              |
| 39:BE:137:HIS:HB3 | 39:BE:138:PRO:HD2  | 2.03                     | 0.41              |
| 40:BF:8:GLN:HB3   | 40:BF:126:VAL:CA   | 2.47                     | 0.41              |
| 48:BP:29:LYS:CD   | 48:BP:29:LYS:N     | 2.82                     | 0.41              |
| 48:BP:48:PRO:C    | 48:BP:50:ARG:N     | 2.74                     | 0.41              |
| 49:BQ:62:GLY:HA3  | 49:BQ:109:VAL:HG22 | 2.03                     | 0.41              |
| 49:BQ:16:ARG:CG   | 49:BQ:16:ARG:NH1   | 2.82                     | 0.41              |
| 52:BT:4:GLY:O     | 52:BT:8:LYS:HB2    | 2.20                     | 0.41              |
| 54:BV:46:VAL:HG13 | 54:BV:46:VAL:O     | 2.21                     | 0.41              |
| 54:BV:3:ALA:HB2   | 54:BV:99:ILE:HG21  | 2.02                     | 0.41              |
| 35:BA:328:U:H4'   | 57:BY:68:HIS:CE1   | 2.56                     | 0.41              |
| 1:AA:1036:G:H2'   | 1:AA:1036:G:N3     | 2.36                     | 0.41              |
| 1:AA:105:G:C6     | 1:AA:106:C:C4      | 3.09                     | 0.41              |
| 1:AA:106:C:O5'    | 1:AA:106:C:H6      | 2.03                     | 0.41              |
| 1:AA:109:A:N3     | 1:AA:109:A:H5''    | 2.36                     | 0.41              |
| 1:AA:1132:C:C4    | 1:AA:1133:G:C6     | 3.08                     | 0.41              |
| 1:AA:114:U:O5'    | 1:AA:114:U:C6      | 2.65                     | 0.41              |
| 1:AA:1384:C:H2'   | 1:AA:1385:G:C5'    | 2.44                     | 0.41              |
| 1:AA:302:G:O2'    | 1:AA:556:C:H5''    | 2.20                     | 0.41              |
| 1:AA:673:G:H2'    | 1:AA:674:G:H8      | 1.73                     | 0.41              |
| 1:AA:683:G:H2'    | 1:AA:684:A:C8      | 2.56                     | 0.41              |
| 1:AA:89:C:N3      | 1:AA:90:U:H5       | 2.18                     | 0.41              |
| 1:AA:1055:A:H2'   | 3:AC:156:ARG:HD2   | 2.03                     | 0.41              |
| 4:AD:4:TYR:HE2    | 4:AD:7:PRO:O       | 2.03                     | 0.41              |
| 5:AE:36:ASP:O     | 5:AE:38:GLN:HG2    | 2.21                     | 0.41              |
| 6:AF:37:VAL:CG1   | 6:AF:38:GLU:N      | 2.84                     | 0.41              |
| 9:AI:122:ALA:HB1  | 9:AI:123:PRO:HD2   | 2.03                     | 0.41              |
| 9:AI:53:VAL:O     | 9:AI:55:ALA:N      | 2.53                     | 0.41              |
| 11:AK:18:ARG:O    | 11:AK:32:ILE:HA    | 2.21                     | 0.41              |
| 11:AK:15:ALA:HB1  | 11:AK:78:GLN:CG    | 2.51                     | 0.41              |
| 15:AO:87:ILE:CG2  | 15:AO:88:ARG:N     | 2.65                     | 0.41              |
| 16:AP:43:LYS:HG3  | 16:AP:48:TRP:CD2   | 2.56                     | 0.41              |
| 17:AQ:65:ILE:N    | 17:AQ:65:ILE:CD1   | 2.83                     | 0.41              |
| 19:AS:42:PRO:HB3  | 19:AS:67:VAL:HG11  | 2.01                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AT:36:LEU:HD12  | 20:AT:55:ILE:HG23  | 2.02                     | 0.41              |
| 22:AV:9:A:C2       | 22:AV:46:G:C6      | 3.09                     | 0.41              |
| 24:AY:461:ILE:HD12 | 24:AY:461:ILE:C    | 2.41                     | 0.41              |
| 24:AY:530:VAL:O    | 24:AY:532:GLY:N    | 2.53                     | 0.41              |
| 24:AY:689:LYS:CG   | 24:AY:690:GLY:N    | 2.83                     | 0.41              |
| 33:B8:38:GLY:O     | 33:B8:42:ARG:CB    | 2.69                     | 0.41              |
| 35:BA:1057:A:H2'   | 35:BA:1058:G:H8    | 1.86                     | 0.41              |
| 35:BA:1215:G:H2'   | 35:BA:1216:G:H5'   | 2.00                     | 0.41              |
| 35:BA:1224:C:C4    | 35:BA:1225:G:C6    | 3.08                     | 0.41              |
| 35:BA:1375:C:H6    | 35:BA:1375:C:O5'   | 2.04                     | 0.41              |
| 35:BA:1445:A:C8    | 35:BA:1460:A:N3    | 2.87                     | 0.41              |
| 35:BA:1595:G:O2'   | 35:BA:1596:A:H5'   | 2.21                     | 0.41              |
| 35:BA:1720:U:H2'   | 35:BA:1721:G:C5'   | 2.19                     | 0.41              |
| 35:BA:1777:U:C2'   | 35:BA:1778:U:H5'   | 2.50                     | 0.41              |
| 35:BA:1819:A:OP1   | 38:BD:158:ALA:HB3  | 2.20                     | 0.41              |
| 1:AA:702:A:N6      | 35:BA:1846:G:OP1   | 2.54                     | 0.41              |
| 35:BA:2133:A:H1'   | 35:BA:2157:G:N2    | 2.35                     | 0.41              |
| 35:BA:469:G:C2'    | 35:BA:470:A:H5''   | 2.51                     | 0.41              |
| 35:BA:49:A:C4'     | 35:BA:50:U:OP2     | 2.57                     | 0.41              |
| 35:BA:522:G:C6     | 35:BA:523:C:C4     | 3.09                     | 0.41              |
| 35:BA:958:U:C6     | 35:BA:958:U:C3'    | 3.04                     | 0.41              |
| 37:BC:117:THR:HG23 | 37:BC:119:ASP:N    | 2.32                     | 0.41              |
| 37:BC:194:ILE:CD1  | 37:BC:227:PRO:CB   | 2.99                     | 0.41              |
| 38:BD:130:ALA:HB2  | 38:BD:192:THR:HB   | 2.03                     | 0.41              |
| 39:BE:9:VAL:HG23   | 52:BT:4:GLY:CA     | 2.42                     | 0.41              |
| 40:BF:4:VAL:HG11   | 40:BF:17:ARG:NE    | 2.36                     | 0.41              |
| 41:BG:166:ASP:O    | 41:BG:170:ARG:HB3  | 2.21                     | 0.41              |
| 41:BG:45:GLU:N     | 41:BG:45:GLU:OE1   | 2.54                     | 0.41              |
| 42:BH:103:LEU:HD23 | 42:BH:148:ILE:HD12 | 2.03                     | 0.41              |
| 42:BH:155:SER:O    | 42:BH:157:TYR:N    | 2.54                     | 0.41              |
| 42:BH:37:VAL:CG1   | 42:BH:38:SER:N     | 2.83                     | 0.41              |
| 49:BQ:21:THR:CG2   | 49:BQ:23:GLY:O     | 2.67                     | 0.41              |
| 50:BR:117:VAL:O    | 50:BR:118:GLU:HB2  | 2.21                     | 0.41              |
| 50:BR:85:PRO:C     | 50:BR:87:TYR:H     | 2.25                     | 0.41              |
| 36:BB:50:G:OP2     | 51:BS:62:LYS:CB    | 2.69                     | 0.41              |
| 54:BV:45:THR:O     | 54:BV:46:VAL:C     | 2.59                     | 0.41              |
| 35:BA:1188:U:C5'   | 54:BV:79:VAL:HG13  | 2.51                     | 0.41              |
| 54:BV:89:GLN:OE1   | 54:BV:89:GLN:HA    | 2.21                     | 0.41              |
| 57:BY:46:LYS:HB3   | 57:BY:62:GLU:HG3   | 2.03                     | 0.41              |
| 58:BZ:153:SER:HB2  | 58:BZ:167:PRO:HG2  | 2.02                     | 0.41              |
| 58:BZ:24:LEU:HA    | 58:BZ:25:PRO:HD2   | 1.96                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:AA:1003:G:N2    | 1:AA:1004:A:H1'     | 2.35                     | 0.41              |
| 1:AA:1258:G:H2'   | 1:AA:1259:C:H6      | 1.85                     | 0.41              |
| 1:AA:1314:C:H5    | 19:AS:6:LYS:HE2     | 1.85                     | 0.41              |
| 1:AA:782:A:O3'    | 1:AA:1515:C:H4'     | 2.21                     | 0.41              |
| 1:AA:1526:G:O2'   | 1:AA:1527:C:C5'     | 2.42                     | 0.41              |
| 1:AA:312:C:H2'    | 1:AA:313:A:O5'      | 2.21                     | 0.41              |
| 1:AA:471:G:C6     | 1:AA:472:A:C5       | 3.09                     | 0.41              |
| 1:AA:718:G:H5'    | 11:AK:117:ASN:CG    | 2.40                     | 0.41              |
| 1:AA:731:G:H5'    | 1:AA:766:A:H4'      | 2.03                     | 0.41              |
| 1:AA:961:U:O2'    | 1:AA:962:C:O5'      | 2.38                     | 0.41              |
| 2:AB:127:ILE:CD1  | 2:AB:135:GLN:NE2    | 2.84                     | 0.41              |
| 4:AD:106:TYR:C    | 4:AD:108:LEU:N      | 2.73                     | 0.41              |
| 8:AH:92:ARG:HD2   | 8:AH:92:ARG:HA      | 1.78                     | 0.41              |
| 11:AK:116:HIS:O   | 11:AK:117:ASN:HB2   | 2.21                     | 0.41              |
| 16:AP:80:PHE:CD1  | 16:AP:80:PHE:N      | 2.89                     | 0.41              |
| 22:AV:43:C:O5'    | 22:AV:43:C:O2       | 2.38                     | 0.41              |
| 25:B0:17:GLN:HA   | 25:B0:17:GLN:NE2    | 2.34                     | 0.41              |
| 25:B0:49:LYS:O    | 25:B0:80:HIS:HB3    | 2.20                     | 0.41              |
| 25:B0:82:ARG:HB3  | 25:B0:82:ARG:HE     | 1.69                     | 0.41              |
| 28:B3:56:VAL:HG12 | 28:B3:57:GLU:N      | 2.36                     | 0.41              |
| 29:B4:1:MET:HB2   | 36:BB:39:A:C6       | 2.56                     | 0.41              |
| 30:B5:7:PRO:HA    | 35:BA:2615:U:C2     | 2.56                     | 0.41              |
| 30:B5:19:ARG:HH12 | 35:BA:1265:A:H3'    | 1.86                     | 0.41              |
| 35:BA:156:U:H2'   | 35:BA:157:U:C5'     | 2.51                     | 0.41              |
| 35:BA:1766:U:H2'  | 35:BA:1767:C:H6     | 1.86                     | 0.41              |
| 35:BA:1892:C:O2'  | 35:BA:1893:C:C5'    | 2.58                     | 0.41              |
| 35:BA:1992:G:C2   | 35:BA:1997:G:C6     | 3.08                     | 0.41              |
| 35:BA:2318:G:C2'  | 35:BA:2319:G:OP1    | 2.69                     | 0.41              |
| 35:BA:2712:U:O2'  | 35:BA:2712(A):A:O5' | 2.39                     | 0.41              |
| 35:BA:271(N):U:P  | 35:BA:271(N):U:H6   | 2.44                     | 0.41              |
| 35:BA:733:G:C8    | 35:BA:761:A:N6      | 2.88                     | 0.41              |
| 35:BA:803:U:O2'   | 35:BA:804:A:H5'     | 2.21                     | 0.41              |
| 35:BA:850:C:O2'   | 35:BA:851:U:H5'     | 2.21                     | 0.41              |
| 37:BC:44:VAL:HG23 | 37:BC:176:VAL:CG2   | 2.51                     | 0.41              |
| 41:BG:36:LYS:HG2  | 41:BG:37:VAL:N      | 2.36                     | 0.41              |
| 42:BH:53:GLU:CG   | 42:BH:54:ARG:N      | 2.84                     | 0.41              |
| 52:BT:19:LEU:HA   | 52:BT:20:PRO:HD3    | 1.74                     | 0.41              |
| 52:BT:42:ILE:HD13 | 52:BT:83:ILE:HD13   | 2.03                     | 0.41              |
| 52:BT:55:ASN:H    | 52:BT:59:THR:HG22   | 1.86                     | 0.41              |
| 54:BV:24:LYS:HA   | 54:BV:92:THR:CG2    | 2.36                     | 0.41              |
| 54:BV:51:VAL:CG1  | 54:BV:52:VAL:N      | 2.80                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:BY:28:LYS:CA   | 57:BY:39:VAL:H     | 2.32                     | 0.41              |
| 1:AA:1125:U:H5    | 10:AJ:73:ASP:OD2   | 2.04                     | 0.40              |
| 1:AA:1256:A:H5'   | 1:AA:1257:U:OP1    | 2.21                     | 0.40              |
| 1:AA:1363:C:H5'   | 1:AA:1363(A):A:O5' | 2.20                     | 0.40              |
| 1:AA:174:C:H2'    | 1:AA:175:C:C6      | 2.56                     | 0.40              |
| 1:AA:434:U:H2'    | 1:AA:435:C:C6      | 2.56                     | 0.40              |
| 1:AA:495:A:C4'    | 1:AA:496:A:C5'     | 2.67                     | 0.40              |
| 1:AA:594:G:C2'    | 1:AA:595:G:H5'     | 2.50                     | 0.40              |
| 1:AA:59:A:H2'     | 1:AA:59:A:N3       | 2.37                     | 0.40              |
| 1:AA:604:G:O2'    | 1:AA:605:U:H5'     | 2.22                     | 0.40              |
| 1:AA:652:U:C2     | 1:AA:752:G:N2      | 2.89                     | 0.40              |
| 1:AA:658:G:O2'    | 1:AA:659:U:H5'     | 2.21                     | 0.40              |
| 1:AA:1193:G:OP1   | 3:AC:167:TRP:HZ3   | 2.04                     | 0.40              |
| 4:AD:60:GLU:O     | 4:AD:63:LYS:HB3    | 2.20                     | 0.40              |
| 8:AH:101:PRO:HG2  | 8:AH:133:LEU:HD21  | 2.02                     | 0.40              |
| 11:AK:124:LYS:NZ  | 11:AK:125:PHE:CE1  | 2.88                     | 0.40              |
| 14:AN:12:ARG:NH1  | 14:AN:12:ARG:HB2   | 2.36                     | 0.40              |
| 14:AN:59:ALA:O    | 14:AN:60:SER:HB2   | 2.20                     | 0.40              |
| 17:AQ:60:ILE:HG21 | 17:AQ:74:LEU:HD23  | 2.02                     | 0.40              |
| 20:AT:69:GLY:O    | 20:AT:73:HIS:HD2   | 2.02                     | 0.40              |
| 20:AT:63:ILE:HG22 | 20:AT:77:ALA:HB1   | 2.04                     | 0.40              |
| 24:AY:238:THR:O   | 24:AY:240:GLU:N    | 2.54                     | 0.40              |
| 24:AY:8:ASP:O     | 24:AY:9:LEU:CB     | 2.69                     | 0.40              |
| 26:B1:3:LYS:CB    | 26:B1:61:ARG:HH21  | 2.33                     | 0.40              |
| 26:B1:53:VAL:O    | 26:B1:54:ALA:C     | 2.59                     | 0.40              |
| 27:B2:10:LEU:HD13 | 35:BA:78:A:P       | 2.60                     | 0.40              |
| 29:B4:40:HIS:HA   | 29:B4:45:GLY:HA3   | 2.03                     | 0.40              |
| 31:B6:51:GLU:O    | 31:B6:52:VAL:CB    | 2.68                     | 0.40              |
| 35:BA:1022:G:C6   | 35:BA:1141:U:C5    | 3.09                     | 0.40              |
| 35:BA:1060:U:O2'  | 35:BA:1061:U:P     | 2.78                     | 0.40              |
| 35:BA:9:U:O2'     | 35:BA:10:G:O5'     | 2.35                     | 0.40              |
| 35:BA:1137:G:C2'  | 35:BA:1138:G:C5'   | 2.96                     | 0.40              |
| 35:BA:1344:G:H5'  | 35:BA:1384:A:C6    | 2.56                     | 0.40              |
| 35:BA:146:G:H8    | 35:BA:146:G:C5'    | 2.29                     | 0.40              |
| 35:BA:1506:C:O2   | 35:BA:1506:C:H2'   | 2.20                     | 0.40              |
| 35:BA:1661:G:C6   | 35:BA:2000:G:C6    | 3.10                     | 0.40              |
| 35:BA:154:G:H1    | 35:BA:172:C:H42    | 1.69                     | 0.40              |
| 35:BA:1779:U:C6   | 35:BA:1779:U:C3'   | 3.04                     | 0.40              |
| 35:BA:1804:C:H2'  | 35:BA:1805:U:H5'   | 2.04                     | 0.40              |
| 35:BA:1805:U:H5'' | 38:BD:250:TRP:CD2  | 2.56                     | 0.40              |
| 35:BA:2523:G:C2'  | 35:BA:2524:G:C5'   | 2.97                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:258:G:H2'    | 35:BA:259:G:H5'    | 2.02                     | 0.40              |
| 35:BA:2629:A:H5'   | 35:BA:2629:A:N3    | 2.36                     | 0.40              |
| 35:BA:271(N):U:P   | 35:BA:271(N):U:C6  | 3.14                     | 0.40              |
| 35:BA:2807:G:H3'   | 35:BA:2808:U:C5'   | 2.41                     | 0.40              |
| 35:BA:2881:C:O2'   | 35:BA:2882:A:H5'   | 2.20                     | 0.40              |
| 35:BA:37:C:C2'     | 35:BA:38:A:C5'     | 2.97                     | 0.40              |
| 35:BA:608:A:H2'    | 35:BA:609:A:C8     | 2.57                     | 0.40              |
| 35:BA:7:G:H2'      | 35:BA:8:A:H8       | 1.85                     | 0.40              |
| 36:BB:111:G:C2'    | 36:BB:112:U:H5'    | 2.50                     | 0.40              |
| 36:BB:13:A:HO2'    | 36:BB:14:U:H3'     | 1.82                     | 0.40              |
| 37:BC:129:GLY:CA   | 37:BC:138:LEU:HD12 | 2.51                     | 0.40              |
| 37:BC:135:ARG:O    | 37:BC:137:LEU:HG   | 2.20                     | 0.40              |
| 37:BC:141:PRO:O    | 37:BC:143:ALA:N    | 2.46                     | 0.40              |
| 37:BC:54:ARG:CZ    | 37:BC:55:SER:O     | 2.69                     | 0.40              |
| 38:BD:210:GLY:C    | 38:BD:212:SER:H    | 2.22                     | 0.40              |
| 39:BE:72:VAL:O     | 39:BE:72:VAL:HG12  | 2.20                     | 0.40              |
| 40:BF:129:PHE:CD2  | 40:BF:163:VAL:HG21 | 2.57                     | 0.40              |
| 42:BH:30:LYS:HG3   | 42:BH:81:GLU:H     | 1.86                     | 0.40              |
| 42:BH:66:GLY:O     | 42:BH:67:LEU:C     | 2.59                     | 0.40              |
| 44:BK:126:UNK:C    | 44:BK:128:UNK:N    | 2.82                     | 0.40              |
| 46:BN:3:THR:O      | 46:BN:4:TYR:CG     | 2.74                     | 0.40              |
| 47:BO:107:ARG:HD3  | 52:BT:36:GLU:CD    | 2.42                     | 0.40              |
| 48:BP:125:VAL:HG13 | 48:BP:125:VAL:O    | 2.21                     | 0.40              |
| 52:BT:35:LYS:NZ    | 52:BT:41:ARG:NE    | 2.69                     | 0.40              |
| 53:BU:39:LEU:HA    | 53:BU:39:LEU:HD23  | 1.94                     | 0.40              |
| 54:BV:47:VAL:HG21  | 54:BV:50:PRO:O     | 2.21                     | 0.40              |
| 54:BV:97:LYS:HD3   | 54:BV:97:LYS:HA    | 1.89                     | 0.40              |
| 55:BW:1:MET:HB3    | 55:BW:64:MET:HE2   | 2.02                     | 0.40              |
| 55:BW:26:GLY:N     | 55:BW:71:VAL:CG2   | 2.84                     | 0.40              |
| 1:AA:1048:G:C2     | 1:AA:1050:G:C5     | 3.10                     | 0.40              |
| 1:AA:951:G:C6      | 1:AA:1231:G:C5     | 3.09                     | 0.40              |
| 1:AA:951:G:C5      | 1:AA:1231:G:C6     | 3.10                     | 0.40              |
| 1:AA:131:C:H2'     | 1:AA:132:C:C6      | 2.56                     | 0.40              |
| 1:AA:1434:A:H2'    | 1:AA:1435:G:O4'    | 2.21                     | 0.40              |
| 1:AA:1496:C:O5'    | 1:AA:1496:C:H6     | 2.04                     | 0.40              |
| 1:AA:443:C:H2'     | 1:AA:444:C:C6      | 2.56                     | 0.40              |
| 1:AA:46:G:H2'      | 1:AA:366:C:C4      | 2.55                     | 0.40              |
| 1:AA:600:C:H2'     | 1:AA:601:C:C6      | 2.56                     | 0.40              |
| 1:AA:890:G:O2'     | 1:AA:906:G:O6      | 2.31                     | 0.40              |
| 1:AA:995:C:O2'     | 1:AA:996:A:P       | 2.80                     | 0.40              |
| 1:AA:995:C:HO2'    | 1:AA:996:A:P       | 2.44                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:185:ILE:HG23 | 2:AB:199:TYR:O    | 2.22                     | 0.40              |
| 3:AC:40:ARG:HG2   | 3:AC:55:VAL:HG11  | 2.03                     | 0.40              |
| 4:AD:169:LYS:HB2  | 4:AD:169:LYS:HE2  | 1.98                     | 0.40              |
| 4:AD:32:ALA:C     | 4:AD:34:GLU:H     | 2.23                     | 0.40              |
| 5:AE:91:LEU:HD12  | 5:AE:91:LEU:HA    | 1.87                     | 0.40              |
| 7:AG:15:ASP:OD1   | 7:AG:16:LEU:N     | 2.54                     | 0.40              |
| 8:AH:23:SER:HB2   | 8:AH:61:VAL:O     | 2.22                     | 0.40              |
| 9:AI:79:LEU:HD13  | 9:AI:83:ARG:HD2   | 2.02                     | 0.40              |
| 1:AA:1149:C:OP2   | 9:AI:9:ARG:NH1    | 2.53                     | 0.40              |
| 11:AK:82:VAL:CG1  | 11:AK:108:ILE:HA  | 2.48                     | 0.40              |
| 12:AL:52:LEU:O    | 12:AL:54:LYS:HD2  | 2.21                     | 0.40              |
| 15:AO:61:GLY:O    | 15:AO:65:ARG:HG2  | 2.22                     | 0.40              |
| 16:AP:53:VAL:O    | 16:AP:57:ARG:HG3  | 2.21                     | 0.40              |
| 24:AY:343:ASN:ND2 | 24:AY:343:ASN:C   | 2.74                     | 0.40              |
| 24:AY:17:ILE:O    | 24:AY:84:THR:HB   | 2.21                     | 0.40              |
| 25:B0:21:LEU:HD11 | 25:B0:41:ARG:HG2  | 2.02                     | 0.40              |
| 25:B0:69:PHE:CE2  | 25:B0:79:VAL:CG2  | 3.03                     | 0.40              |
| 26:B1:11:ARG:NH1  | 26:B1:11:ARG:CG   | 2.81                     | 0.40              |
| 28:B3:31:LEU:HD23 | 28:B3:31:LEU:HA   | 1.85                     | 0.40              |
| 29:B4:56:VAL:CG2  | 29:B4:57:GLU:N    | 2.80                     | 0.40              |
| 30:B5:47:PRO:HG2  | 30:B5:48:GLU:H    | 1.85                     | 0.40              |
| 31:B6:15:GLU:OE1  | 31:B6:18:ARG:HG2  | 2.21                     | 0.40              |
| 33:B8:62:LEU:HG   | 33:B8:62:LEU:H    | 1.69                     | 0.40              |
| 35:BA:1009:A:H5'  | 53:BU:59:ARG:HD3  | 2.03                     | 0.40              |
| 35:BA:1131:G:N2   | 46:BN:73:THR:CG2  | 2.84                     | 0.40              |
| 35:BA:118:A:OP2   | 35:BA:119:A:H5''  | 2.21                     | 0.40              |
| 35:BA:1415:U:HO2' | 35:BA:1417:C:P    | 2.43                     | 0.40              |
| 35:BA:145:G:C2'   | 35:BA:146:G:C5'   | 2.82                     | 0.40              |
| 35:BA:1503:U:C2   | 35:BA:1504:C:C5   | 3.10                     | 0.40              |
| 35:BA:1697:G:C2'  | 35:BA:1698:A:OP1  | 2.69                     | 0.40              |
| 35:BA:16:G:H2'    | 35:BA:17:G:C5'    | 2.50                     | 0.40              |
| 35:BA:1765:C:H2'  | 35:BA:1766:U:H6   | 1.86                     | 0.40              |
| 35:BA:2038:G:H2'  | 35:BA:2039:C:O4'  | 2.21                     | 0.40              |
| 35:BA:2297:C:O2'  | 35:BA:2298:A:H5'  | 2.21                     | 0.40              |
| 35:BA:2403:C:H2'  | 35:BA:2404:C:H5'  | 2.03                     | 0.40              |
| 35:BA:2672:G:H3'  | 35:BA:2673:G:H5'' | 2.03                     | 0.40              |
| 35:BA:2752:C:H2'  | 35:BA:2753:A:H5'  | 2.03                     | 0.40              |
| 35:BA:2771:C:H2'  | 35:BA:2772:C:C6   | 2.55                     | 0.40              |
| 35:BA:860:U:C5    | 35:BA:917:A:N7    | 2.82                     | 0.40              |
| 35:BA:923:C:H2'   | 35:BA:924:C:C6    | 2.56                     | 0.40              |
| 37:BC:98:GLU:O    | 37:BC:99:GLU:C    | 2.59                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:BE:1:MET:O     | 39:BE:2:LYS:O      | 2.40                     | 0.40              |
| 41:BG:83:ARG:HB2  | 41:BG:84:LYS:H     | 1.51                     | 0.40              |
| 42:BH:90:LYS:HD2  | 42:BH:163:TYR:CE1  | 2.55                     | 0.40              |
| 44:BK:95:UNK:O    | 44:BK:96:UNK:O     | 2.38                     | 0.40              |
| 35:BA:389:G:C6    | 48:BP:70:GLN:HG3   | 2.55                     | 0.40              |
| 50:BR:76:VAL:O    | 50:BR:79:LEU:HB3   | 2.22                     | 0.40              |
| 51:BS:33:LYS:HB3  | 51:BS:34:HIS:HD2   | 1.86                     | 0.40              |
| 52:BT:33:LYS:NZ   | 52:BT:43:GLN:NE2   | 2.68                     | 0.40              |
| 56:BX:13:LEU:O    | 56:BX:14:SER:HB3   | 2.21                     | 0.40              |
| 1:AA:1179:A:H2'   | 1:AA:1180:A:O4'    | 2.21                     | 0.40              |
| 1:AA:1452:C:OP1   | 1:AA:1452:C:C6     | 2.74                     | 0.40              |
| 1:AA:443:C:H2'    | 1:AA:444:C:H6      | 1.86                     | 0.40              |
| 1:AA:546:G:O2'    | 1:AA:547:A:O5'     | 2.30                     | 0.40              |
| 1:AA:589:C:H2'    | 1:AA:590:C:H5'     | 2.02                     | 0.40              |
| 1:AA:744:C:H2'    | 1:AA:745:C:H6      | 1.87                     | 0.40              |
| 1:AA:992:U:O2'    | 1:AA:993:G:P       | 2.80                     | 0.40              |
| 2:AB:24:TRP:CE3   | 2:AB:32:ILE:HD12   | 2.54                     | 0.40              |
| 2:AB:26:PRO:O     | 2:AB:29:ALA:HB2    | 2.21                     | 0.40              |
| 3:AC:103:VAL:CG1  | 3:AC:104:GLN:N     | 2.84                     | 0.40              |
| 3:AC:134:ILE:HD11 | 3:AC:153:VAL:HG23  | 2.03                     | 0.40              |
| 3:AC:31:HIS:O     | 3:AC:32:LEU:C      | 2.60                     | 0.40              |
| 4:AD:101:LEU:O    | 4:AD:102:ASP:C     | 2.60                     | 0.40              |
| 8:AH:100:ILE:HG22 | 8:AH:125:ARG:HH12  | 1.87                     | 0.40              |
| 9:AI:117:HIS:C    | 9:AI:118:LYS:CG    | 2.89                     | 0.40              |
| 10:AJ:44:VAL:HG22 | 10:AJ:66:ARG:CG    | 2.42                     | 0.40              |
| 11:AK:50:TYR:O    | 11:AK:51:LYS:HG3   | 2.21                     | 0.40              |
| 12:AL:45:PRO:HD2  | 12:AL:51:ALA:O     | 2.19                     | 0.40              |
| 1:AA:1307:U:O4'   | 13:AM:109:THR:HG21 | 2.21                     | 0.40              |
| 24:AY:242:LEU:O   | 24:AY:245:ALA:HB3  | 2.22                     | 0.40              |
| 24:AY:401:SER:O   | 24:AY:402:ILE:HB   | 2.21                     | 0.40              |
| 24:AY:568:TYR:HD1 | 24:AY:568:TYR:H    | 1.70                     | 0.40              |
| 35:BA:1351:C:O2'  | 35:BA:1571:A:H1'   | 2.21                     | 0.40              |
| 35:BA:1530:C:H2'  | 35:BA:1531:C:H6    | 1.86                     | 0.40              |
| 35:BA:1973:G:O2'  | 35:BA:1974:C:H5'   | 2.22                     | 0.40              |
| 35:BA:2011:U:C2'  | 35:BA:2012:G:C5'   | 3.00                     | 0.40              |
| 35:BA:2100:G:H2'  | 35:BA:2100:G:N3    | 2.36                     | 0.40              |
| 35:BA:2117:A:HO2' | 35:BA:2118:U:H3'   | 1.83                     | 0.40              |
| 35:BA:2552:U:C2   | 35:BA:2554:U:H5'   | 2.56                     | 0.40              |
| 35:BA:1956:U:H1'  | 35:BA:2552:U:OP1   | 2.21                     | 0.40              |
| 35:BA:2588:G:O6   | 35:BA:2607:G:C6    | 2.75                     | 0.40              |
| 35:BA:265:A:O4'   | 35:BA:266:G:O4'    | 2.39                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:303:U:O2'   | 35:BA:304:G:H5'    | 2.21                     | 0.40              |
| 35:BA:373:U:H2'   | 35:BA:374:A:H8     | 1.87                     | 0.40              |
| 35:BA:813:U:H2'   | 35:BA:814:C:C6     | 2.56                     | 0.40              |
| 35:BA:815:C:H2'   | 35:BA:816:C:H6     | 1.85                     | 0.40              |
| 37:BC:228:HIS:O   | 37:BC:229:SER:CB   | 2.68                     | 0.40              |
| 35:BA:1902:C:C3'  | 38:BD:244:ARG:HB2  | 2.51                     | 0.40              |
| 40:BF:46:ARG:HG3  | 40:BF:48:THR:HG23  | 2.04                     | 0.40              |
| 36:BB:56:G:H5''   | 41:BG:27:ASN:HD21  | 1.83                     | 0.40              |
| 41:BG:45:GLU:OE2  | 41:BG:152:LEU:HD11 | 2.21                     | 0.40              |
| 42:BH:30:LYS:HZ2  | 42:BH:30:LYS:HG2   | 1.74                     | 0.40              |
| 46:BN:119:ARG:CG  | 46:BN:119:ARG:NH1  | 2.83                     | 0.40              |
| 47:BO:1:MET:HB3   | 47:BO:32:TYR:CD2   | 2.56                     | 0.40              |
| 48:BP:6:LEU:CD1   | 48:BP:9:ASN:OD1    | 2.67                     | 0.40              |
| 58:BZ:29:TYR:O    | 58:BZ:30:ASN:HB3   | 2.21                     | 0.40              |
| 58:BZ:30:ASN:HB3  | 58:BZ:89:PHE:CE1   | 2.56                     | 0.40              |
| 1:AA:1154:G:C2    | 1:AA:1155:G:C8     | 3.10                     | 0.40              |
| 1:AA:1118:C:H1'   | 1:AA:1179:A:C8     | 2.56                     | 0.40              |
| 1:AA:1437:C:O2'   | 1:AA:1438:G:H5'    | 2.21                     | 0.40              |
| 1:AA:165:C:O2'    | 1:AA:166:G:H5'     | 2.20                     | 0.40              |
| 1:AA:89:C:C1'     | 1:AA:90:U:OP1      | 2.66                     | 0.40              |
| 1:AA:935:A:H2'    | 1:AA:936:C:C6      | 2.56                     | 0.40              |
| 1:AA:937:A:C5     | 1:AA:938:A:N7      | 2.90                     | 0.40              |
| 2:AB:127:ILE:HD13 | 2:AB:135:GLN:HE21  | 1.86                     | 0.40              |
| 2:AB:189:ASP:OD1  | 2:AB:189:ASP:N     | 2.55                     | 0.40              |
| 3:AC:121:ALA:HB1  | 3:AC:198:VAL:HG21  | 2.02                     | 0.40              |
| 8:AH:36:LEU:O     | 8:AH:37:ARG:C      | 2.59                     | 0.40              |
| 8:AH:34:GLU:OE1   | 8:AH:37:ARG:NH1    | 2.55                     | 0.40              |
| 13:AM:22:ILE:HG22 | 13:AM:23:TYR:N     | 2.37                     | 0.40              |
| 1:AA:1316:G:O3'   | 14:AN:18:VAL:CG1   | 2.70                     | 0.40              |
| 15:AO:82:ILE:HD13 | 15:AO:82:ILE:C     | 2.41                     | 0.40              |
| 6:AF:91:VAL:HG13  | 18:AR:72:ARG:NH2   | 2.36                     | 0.40              |
| 20:AT:39:LYS:HE3  | 20:AT:39:LYS:HB2   | 1.93                     | 0.40              |
| 24:AY:247:ARG:O   | 24:AY:251:ILE:HG13 | 2.21                     | 0.40              |
| 24:AY:507:TYR:CD1 | 24:AY:507:TYR:C    | 2.94                     | 0.40              |
| 26:B1:30:VAL:H    | 35:BA:2396:G:H4'   | 1.87                     | 0.40              |
| 27:B2:39:ALA:C    | 27:B2:41:ILE:N     | 2.74                     | 0.40              |
| 28:B3:4:LEU:HG    | 28:B3:39:ASP:HB2   | 2.02                     | 0.40              |
| 33:B8:15:LYS:CD   | 48:BP:65:ARG:NH2   | 2.79                     | 0.40              |
| 35:BA:1093:G:H1'  | 35:BA:1099:G:N2    | 2.33                     | 0.40              |
| 35:BA:1103:A:H5'  | 35:BA:1104:C:H5    | 1.85                     | 0.40              |
| 35:BA:1161:C:O2'  | 54:BV:23:GLU:HG3   | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1199:U:H2'   | 35:BA:1200:C:O4'   | 2.21                     | 0.40              |
| 35:BA:1216:G:C2'   | 35:BA:1217:C:C5'   | 2.95                     | 0.40              |
| 35:BA:1273:U:C5'   | 35:BA:1646:C:H41   | 2.31                     | 0.40              |
| 35:BA:1683:C:H2'   | 35:BA:1684:C:H6    | 1.85                     | 0.40              |
| 35:BA:1798:U:H5'   | 38:BD:259:THR:CG2  | 2.46                     | 0.40              |
| 35:BA:2104:G:C1'   | 35:BA:2105:C:OP1   | 2.64                     | 0.40              |
| 35:BA:2199:A:H5''  | 35:BA:2200:C:OP2   | 2.20                     | 0.40              |
| 35:BA:2252:G:H2'   | 35:BA:2253:G:C8    | 2.57                     | 0.40              |
| 35:BA:2252:G:O2'   | 35:BA:2253:G:H5'   | 2.22                     | 0.40              |
| 24:AY:87:HIS:NE2   | 35:BA:2662:A:OP1   | 2.48                     | 0.40              |
| 35:BA:265:A:H4'    | 35:BA:266:G:O5'    | 2.22                     | 0.40              |
| 35:BA:57:C:H2'     | 35:BA:58:G:O4'     | 2.20                     | 0.40              |
| 35:BA:911:A:O5'    | 35:BA:911:A:H8     | 2.04                     | 0.40              |
| 35:BA:967:C:H2'    | 35:BA:968:G:H8     | 1.86                     | 0.40              |
| 41:BG:40:ASN:CG    | 41:BG:91:ARG:HB2   | 2.42                     | 0.40              |
| 41:BG:73:ALA:HB3   | 41:BG:85:GLY:CA    | 2.50                     | 0.40              |
| 44:BK:95:UNK:O     | 44:BK:96:UNK:C     | 2.70                     | 0.40              |
| 46:BN:74:ARG:HH21  | 46:BN:83:LYS:HD3   | 1.85                     | 0.40              |
| 47:BO:24:VAL:O     | 47:BO:24:VAL:CG2   | 2.70                     | 0.40              |
| 47:BO:48:PRO:O     | 47:BO:49:ARG:C     | 2.59                     | 0.40              |
| 48:BP:95:VAL:HB    | 48:BP:100:LEU:HD21 | 2.03                     | 0.40              |
| 51:BS:52:SER:HB3   | 51:BS:55:ALA:HB3   | 2.02                     | 0.40              |
| 53:BU:18:LEU:HD13  | 53:BU:18:LEU:HA    | 1.96                     | 0.40              |
| 53:BU:57:PHE:C     | 53:BU:59:ARG:N     | 2.71                     | 0.40              |
| 55:BW:5:ALA:CB     | 55:BW:50:VAL:HG23  | 2.52                     | 0.40              |
| 27:B2:36:ARG:NH2   | 56:BX:5:TYR:O      | 2.39                     | 0.40              |
| 57:BY:2:ARG:O      | 57:BY:3:VAL:CB     | 2.69                     | 0.40              |
| 57:BY:3:VAL:C      | 57:BY:5:MET:N      | 2.74                     | 0.40              |
| 58:BZ:151:HIS:HB2  | 58:BZ:170:THR:CA   | 2.38                     | 0.40              |
| 1:AA:1007:C:O2'    | 1:AA:1008:C:H5'    | 2.20                     | 0.40              |
| 1:AA:1030(D):A:H1' | 1:AA:1031:G:OP2    | 2.21                     | 0.40              |
| 1:AA:1151:A:N3     | 1:AA:1152:A:C8     | 2.89                     | 0.40              |
| 1:AA:34:C:H2'      | 1:AA:35:G:H8       | 1.86                     | 0.40              |
| 1:AA:414:A:C2      | 1:AA:415:A:C4      | 3.09                     | 0.40              |
| 1:AA:60:A:H62      | 1:AA:110:C:N4      | 2.19                     | 0.40              |
| 1:AA:678:U:H2'     | 1:AA:679:C:C6      | 2.57                     | 0.40              |
| 1:AA:689:C:O2'     | 1:AA:690:G:H5'     | 2.21                     | 0.40              |
| 1:AA:737:A:H2'     | 1:AA:738:C:C6      | 2.57                     | 0.40              |
| 1:AA:8:A:H5'       | 5:AE:120:THR:O     | 2.21                     | 0.40              |
| 1:AA:89:C:C4       | 1:AA:90:U:H5       | 2.40                     | 0.40              |
| 2:AB:111:ARG:NH2   | 2:AB:114:ARG:HG2   | 2.36                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:137:ARG:O     | 2:AB:137:ARG:HD3   | 2.21                     | 0.40              |
| 2:AB:167:PRO:HG3   | 2:AB:188:ALA:CB    | 2.50                     | 0.40              |
| 2:AB:213:LEU:HD23  | 2:AB:217:ARG:HG2   | 2.03                     | 0.40              |
| 2:AB:95:GLN:OE1    | 2:AB:95:GLN:HA     | 2.21                     | 0.40              |
| 5:AE:145:LYS:HA    | 8:AH:107:LEU:CD2   | 2.52                     | 0.40              |
| 5:AE:28:PHE:N      | 5:AE:28:PHE:CD1    | 2.90                     | 0.40              |
| 7:AG:64:GLN:HG3    | 7:AG:128:ALA:O     | 2.21                     | 0.40              |
| 8:AH:100:ILE:HB    | 8:AH:125:ARG:NH1   | 2.37                     | 0.40              |
| 13:AM:52:GLU:HA    | 13:AM:55:ARG:HD3   | 2.03                     | 0.40              |
| 17:AQ:59:ILE:HG22  | 17:AQ:71:PHE:HD2   | 1.84                     | 0.40              |
| 17:AQ:66:SER:OG    | 17:AQ:69:LYS:HB2   | 2.21                     | 0.40              |
| 19:AS:51:VAL:CG2   | 19:AS:71:LEU:HB3   | 2.51                     | 0.40              |
| 22:AV:46:G:H3'     | 22:AV:47:U:C5'     | 2.51                     | 0.40              |
| 24:AY:100:VAL:HG21 | 24:AY:314:PHE:CD1  | 2.55                     | 0.40              |
| 24:AY:192:LEU:HD12 | 24:AY:194:THR:CG2  | 2.49                     | 0.40              |
| 24:AY:199:ILE:H    | 24:AY:199:ILE:HG13 | 1.72                     | 0.40              |
| 24:AY:506:GLN:HB3  | 24:AY:507:TYR:H    | 1.70                     | 0.40              |
| 24:AY:25:LYS:HZ2   | 24:AY:86:GLY:CA    | 2.34                     | 0.40              |
| 25:B0:25:ARG:HD2   | 25:B0:29:GLN:NE2   | 2.37                     | 0.40              |
| 27:B2:10:LEU:HB3   | 27:B2:14:ARG:CZ    | 2.51                     | 0.40              |
| 29:B4:28:LYS:HZ2   | 41:BG:145:THR:N    | 2.19                     | 0.40              |
| 33:B8:26:LYS:CB    | 33:B8:44:LYS:HG3   | 2.51                     | 0.40              |
| 35:BA:1228:G:C2    | 35:BA:1229:G:N9    | 2.89                     | 0.40              |
| 35:BA:1418:G:O5'   | 35:BA:1418:G:H8    | 2.04                     | 0.40              |
| 35:BA:156:U:H2'    | 35:BA:157:U:H5'    | 2.04                     | 0.40              |
| 35:BA:2026:C:H2'   | 35:BA:2027:G:O4'   | 2.22                     | 0.40              |
| 35:BA:2105:C:P     | 35:BA:2105:C:O4'   | 2.80                     | 0.40              |
| 35:BA:2117:A:O2'   | 35:BA:2118:U:P     | 2.80                     | 0.40              |
| 35:BA:246:C:C2'    | 35:BA:247:G:H5''   | 2.45                     | 0.40              |
| 35:BA:2061:G:H5''  | 35:BA:2503:A:C2    | 2.55                     | 0.40              |
| 35:BA:2564:A:C2    | 35:BA:2647:U:H4'   | 2.57                     | 0.40              |
| 35:BA:2712:U:C1'   | 35:BA:2712(A):A:N7 | 2.84                     | 0.40              |
| 35:BA:2801:A:O2'   | 35:BA:2894:G:H5''  | 2.21                     | 0.40              |
| 35:BA:492:A:H2'    | 35:BA:493:G:H5'    | 2.03                     | 0.40              |
| 35:BA:545:C:OP1    | 35:BA:545:C:H6     | 2.04                     | 0.40              |
| 35:BA:848:G:C4     | 35:BA:933:A:C8     | 3.09                     | 0.40              |
| 35:BA:896:A:C8     | 58:BZ:146:ILE:CD1  | 3.05                     | 0.40              |
| 35:BA:953:A:C2     | 35:BA:954:G:C8     | 3.10                     | 0.40              |
| 36:BB:22:U:O2'     | 36:BB:23:G:H5'     | 2.21                     | 0.40              |
| 36:BB:93:G:H2'     | 36:BB:94:C:C6      | 2.56                     | 0.40              |
| 37:BC:89:GLU:O     | 37:BC:90:ALA:HB3   | 2.20                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:BD:165:ILE:HG23 | 38:BD:173:VAL:CG2 | 2.52                     | 0.40              |
| 39:BE:137:HIS:CB   | 39:BE:138:PRO:HD2 | 2.51                     | 0.40              |
| 41:BG:106:LEU:CA   | 41:BG:110:ALA:HB3 | 2.52                     | 0.40              |
| 41:BG:43:LEU:HD13  | 41:BG:48:GLU:H    | 1.87                     | 0.40              |
| 42:BH:84:SER:O     | 42:BH:85:LYS:HB3  | 2.22                     | 0.40              |
| 43:BJ:17:UNK:C     | 43:BJ:19:UNK:N    | 2.85                     | 0.40              |
| 48:BP:121:LYS:O    | 48:BP:123:LEU:CD2 | 2.61                     | 0.40              |
| 51:BS:11:LYS:C     | 51:BS:13:ARG:N    | 2.74                     | 0.40              |
| 56:BX:40:LYS:O     | 56:BX:44:GLU:HG3  | 2.20                     | 0.40              |

All (40) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1            | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------------|--------------------------|-------------------|
| 20:AT:100:ILE:CG1 | 27:B2:43:GLN:CD[2_554]  | 0.34                     | 1.86              |
| 20:AT:100:ILE:CD1 | 27:B2:43:GLN:NE2[2_554] | 0.69                     | 1.51              |
| 3:AC:79:ARG:CD    | 35:BA:2139:C:C4[2_555]  | 0.83                     | 1.37              |
| 3:AC:79:ARG:CD    | 35:BA:2139:C:C5[2_555]  | 0.87                     | 1.33              |
| 3:AC:79:ARG:CG    | 35:BA:2139:C:C6[2_555]  | 0.96                     | 1.24              |
| 3:AC:79:ARG:CZ    | 35:BA:2139:C:N4[2_555]  | 1.08                     | 1.12              |
| 20:AT:100:ILE:CB  | 27:B2:43:GLN:OE1[2_554] | 1.11                     | 1.09              |
| 3:AC:79:ARG:NE    | 35:BA:2139:C:C4[2_555]  | 1.16                     | 1.04              |
| 3:AC:79:ARG:NH1   | 35:BA:2139:C:N4[2_555]  | 1.19                     | 1.01              |
| 20:AT:100:ILE:CG2 | 27:B2:43:GLN:OE1[2_554] | 1.21                     | 0.99              |
| 3:AC:79:ARG:CG    | 35:BA:2139:C:N1[2_555]  | 1.24                     | 0.96              |
| 3:AC:79:ARG:NE    | 35:BA:2139:C:N4[2_555]  | 1.32                     | 0.88              |
| 20:AT:100:ILE:CG1 | 27:B2:43:GLN:OE1[2_554] | 1.33                     | 0.87              |
| 3:AC:79:ARG:CG    | 35:BA:2139:C:C5[2_555]  | 1.42                     | 0.78              |
| 20:AT:100:ILE:CG1 | 27:B2:43:GLN:CG[2_554]  | 1.43                     | 0.77              |
| 20:AT:100:ILE:CG1 | 27:B2:43:GLN:NE2[2_554] | 1.43                     | 0.77              |
| 20:AT:100:ILE:CD1 | 27:B2:43:GLN:CD[2_554]  | 1.48                     | 0.72              |
| 3:AC:81:GLY:N     | 35:BA:2140:C:OP2[2_555] | 1.54                     | 0.66              |
| 20:AT:100:ILE:CB  | 27:B2:43:GLN:CD[2_554]  | 1.60                     | 0.60              |
| 3:AC:79:ARG:NE    | 35:BA:2139:C:N3[2_555]  | 1.61                     | 0.59              |
| 3:AC:78:GLY:O     | 35:BA:2140:C:O4'[2_555] | 1.71                     | 0.49              |
| 3:AC:77:ILE:O     | 35:BA:2140:C:OP1[2_555] | 1.71                     | 0.49              |
| 3:AC:79:ARG:N     | 35:BA:2139:C:C3'[2_555] | 1.71                     | 0.49              |
| 3:AC:79:ARG:CD    | 35:BA:2139:C:N4[2_555]  | 1.76                     | 0.44              |
| 3:AC:79:ARG:N     | 35:BA:2139:C:C2'[2_555] | 1.77                     | 0.43              |
| 3:AC:79:ARG:CG    | 35:BA:2139:C:C2[2_555]  | 1.86                     | 0.34              |

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| Atom-1            | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------------|--------------------------|-------------------|
| 3:AC:79:ARG:CD    | 35:BA:2139:C:C6[2_555]  | 1.92                     | 0.28              |
| 3:AC:79:ARG:CG    | 35:BA:2139:C:C4[2_555]  | 1.93                     | 0.27              |
| 3:AC:79:ARG:CD    | 35:BA:2139:C:N3[2_555]  | 1.93                     | 0.27              |
| 3:AC:78:GLY:C     | 35:BA:2140:C:O5'[2_555] | 1.93                     | 0.27              |
| 3:AC:80:GLY:N     | 35:BA:2139:C:O3'[2_555] | 2.01                     | 0.19              |
| 3:AC:78:GLY:O     | 35:BA:2140:C:O5'[2_555] | 2.02                     | 0.18              |
| 3:AC:79:ARG:CZ    | 35:BA:2139:C:C4[2_555]  | 2.06                     | 0.14              |
| 3:AC:78:GLY:CA    | 35:BA:2140:C:OP1[2_555] | 2.08                     | 0.12              |
| 20:AT:100:ILE:CD1 | 27:B2:43:GLN:CG[2_554]  | 2.09                     | 0.11              |
| 3:AC:79:ARG:NH1   | 35:BA:2152:G:N1[2_555]  | 2.11                     | 0.09              |
| 3:AC:79:ARG:CB    | 35:BA:2139:C:C6[2_555]  | 2.12                     | 0.08              |
| 20:AT:100:ILE:CB  | 27:B2:43:GLN:NE2[2_554] | 2.12                     | 0.08              |
| 3:AC:79:ARG:CG    | 35:BA:2139:C:N3[2_555]  | 2.12                     | 0.08              |
| 2:AB:105:PHE:CE2  | 37:BC:28:ARG:NH2[2_555] | 2.16                     | 0.04              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | AB    | 233/256 (91%) | 163 (70%) | 44 (19%) | 26 (11%) | 0           | 2  |
| 3   | AC    | 205/239 (86%) | 145 (71%) | 32 (16%) | 28 (14%) | 0           | 1  |
| 4   | AD    | 206/209 (99%) | 160 (78%) | 35 (17%) | 11 (5%)  | 2           | 11 |
| 5   | AE    | 149/162 (92%) | 134 (90%) | 12 (8%)  | 3 (2%)   | 9           | 36 |
| 6   | AF    | 99/101 (98%)  | 80 (81%)  | 13 (13%) | 6 (6%)   | 2           | 8  |
| 7   | AG    | 153/156 (98%) | 113 (74%) | 26 (17%) | 14 (9%)  | 1           | 3  |
| 8   | AH    | 136/138 (99%) | 122 (90%) | 13 (10%) | 1 (1%)   | 25          | 64 |
| 9   | AI    | 125/128 (98%) | 93 (74%)  | 21 (17%) | 11 (9%)  | 1           | 3  |
| 10  | AJ    | 97/105 (92%)  | 73 (75%)  | 15 (16%) | 9 (9%)   | 1           | 3  |
| 11  | AK    | 117/129 (91%) | 95 (81%)  | 19 (16%) | 3 (3%)   | 6           | 28 |
| 12  | AL    | 123/132 (93%) | 101 (82%) | 11 (9%)  | 11 (9%)  | 1           | 3  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 13  | AM    | 117/126 (93%) | 74 (63%)  | 32 (27%) | 11 (9%)  | 1           | 3   |
| 14  | AN    | 58/61 (95%)   | 44 (76%)  | 7 (12%)  | 7 (12%)  | 0           | 1   |
| 15  | AO    | 86/89 (97%)   | 78 (91%)  | 7 (8%)   | 1 (1%)   | 15          | 50  |
| 16  | AP    | 82/88 (93%)   | 73 (89%)  | 7 (8%)   | 2 (2%)   | 7           | 31  |
| 17  | AQ    | 98/105 (93%)  | 86 (88%)  | 10 (10%) | 2 (2%)   | 9           | 36  |
| 18  | AR    | 68/88 (77%)   | 58 (85%)  | 8 (12%)  | 2 (3%)   | 5           | 25  |
| 19  | AS    | 86/93 (92%)   | 53 (62%)  | 21 (24%) | 12 (14%) | 0           | 1   |
| 20  | AT    | 97/106 (92%)  | 79 (81%)  | 10 (10%) | 8 (8%)   | 1           | 4   |
| 21  | AU    | 23/27 (85%)   | 17 (74%)  | 4 (17%)  | 2 (9%)   | 1           | 3   |
| 24  | AY    | 685/691 (99%) | 537 (78%) | 99 (14%) | 49 (7%)  | 1           | 5   |
| 25  | B0    | 82/84 (98%)   | 56 (68%)  | 19 (23%) | 7 (8%)   | 1           | 4   |
| 26  | B1    | 92/97 (95%)   | 73 (79%)  | 14 (15%) | 5 (5%)   | 2           | 11  |
| 27  | B2    | 69/71 (97%)   | 45 (65%)  | 11 (16%) | 13 (19%) | 0           | 0   |
| 28  | B3    | 58/60 (97%)   | 50 (86%)  | 7 (12%)  | 1 (2%)   | 11          | 41  |
| 29  | B4    | 69/71 (97%)   | 16 (23%)  | 17 (25%) | 36 (52%) | 0           | 0   |
| 30  | B5    | 57/59 (97%)   | 45 (79%)  | 3 (5%)   | 9 (16%)  | 0           | 1   |
| 31  | B6    | 48/53 (91%)   | 22 (46%)  | 11 (23%) | 15 (31%) | 0           | 0   |
| 32  | B7    | 46/48 (96%)   | 43 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 33  | B8    | 62/64 (97%)   | 42 (68%)  | 8 (13%)  | 12 (19%) | 0           | 0   |
| 34  | B9    | 35/37 (95%)   | 23 (66%)  | 9 (26%)  | 3 (9%)   | 1           | 3   |
| 37  | BC    | 225/228 (99%) | 121 (54%) | 56 (25%) | 48 (21%) | 0           | 0   |
| 38  | BD    | 273/275 (99%) | 222 (81%) | 33 (12%) | 18 (7%)  | 1           | 6   |
| 39  | BE    | 203/206 (98%) | 145 (71%) | 34 (17%) | 24 (12%) | 0           | 1   |
| 40  | BF    | 206/210 (98%) | 165 (80%) | 19 (9%)  | 22 (11%) | 0           | 2   |
| 41  | BG    | 177/181 (98%) | 78 (44%)  | 49 (28%) | 50 (28%) | 0           | 0   |
| 42  | BH    | 174/180 (97%) | 112 (64%) | 31 (18%) | 31 (18%) | 0           | 0   |
| 43  | BJ    | 1/130 (1%)    | 0         | 1 (100%) | 0        | 100         | 100 |
| 46  | BN    | 137/140 (98%) | 110 (80%) | 15 (11%) | 12 (9%)  | 1           | 3   |
| 47  | BO    | 120/122 (98%) | 109 (91%) | 8 (7%)   | 3 (2%)   | 6           | 29  |
| 48  | BP    | 144/149 (97%) | 84 (58%)  | 23 (16%) | 37 (26%) | 0           | 0   |
| 49  | BQ    | 139/141 (99%) | 115 (83%) | 18 (13%) | 6 (4%)   | 3           | 15  |

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| Mol | Chain | Analysed        | Favoured   | Allowed    | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|------------|-----------|-------------|----|
| 50  | BR    | 115/117 (98%)   | 90 (78%)   | 17 (15%)   | 8 (7%)    | 1           | 5  |
| 51  | BS    | 97/111 (87%)    | 52 (54%)   | 25 (26%)   | 20 (21%)  | 0           | 0  |
| 52  | BT    | 136/146 (93%)   | 90 (66%)   | 25 (18%)   | 21 (15%)  | 0           | 1  |
| 53  | BU    | 115/117 (98%)   | 87 (76%)   | 22 (19%)   | 6 (5%)    | 2           | 11 |
| 54  | BV    | 99/101 (98%)    | 73 (74%)   | 11 (11%)   | 15 (15%)  | 0           | 1  |
| 55  | BW    | 111/113 (98%)   | 93 (84%)   | 14 (13%)   | 4 (4%)    | 4           | 19 |
| 56  | BX    | 91/95 (96%)     | 79 (87%)   | 11 (12%)   | 1 (1%)    | 17          | 53 |
| 57  | BY    | 99/109 (91%)    | 54 (54%)   | 17 (17%)   | 28 (28%)  | 0           | 0  |
| 58  | BZ    | 183/205 (89%)   | 131 (72%)  | 30 (16%)   | 22 (12%)  | 0           | 1  |
| All | All   | 6506/6949 (94%) | 4803 (74%) | 1007 (16%) | 696 (11%) | 0           | 2  |

All (696) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 15  | VAL  |
| 2   | AB    | 26  | PRO  |
| 2   | AB    | 37  | ASN  |
| 2   | AB    | 76  | GLN  |
| 2   | AB    | 77  | ALA  |
| 2   | AB    | 150 | SER  |
| 2   | AB    | 191 | ASP  |
| 2   | AB    | 229 | VAL  |
| 2   | AB    | 231 | GLU  |
| 3   | AC    | 12  | LEU  |
| 3   | AC    | 82  | GLU  |
| 3   | AC    | 84  | ILE  |
| 3   | AC    | 119 | ARG  |
| 3   | AC    | 131 | ARG  |
| 3   | AC    | 160 | ALA  |
| 3   | AC    | 169 | ALA  |
| 3   | AC    | 188 | LEU  |
| 4   | AD    | 35  | ARG  |
| 6   | AF    | 87  | ARG  |
| 7   | AG    | 7   | ALA  |
| 7   | AG    | 8   | GLU  |
| 7   | AG    | 50  | ILE  |
| 7   | AG    | 77  | SER  |
| 7   | AG    | 87  | VAL  |
| 7   | AG    | 88  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | AI    | 23  | ASN  |
| 9   | AI    | 25  | LYS  |
| 9   | AI    | 26  | VAL  |
| 9   | AI    | 56  | LEU  |
| 9   | AI    | 118 | LYS  |
| 10  | AJ    | 36  | GLY  |
| 10  | AJ    | 90  | LEU  |
| 11  | AK    | 48  | ILE  |
| 12  | AL    | 27  | LEU  |
| 12  | AL    | 28  | LYS  |
| 12  | AL    | 47  | LYS  |
| 12  | AL    | 94  | PRO  |
| 13  | AM    | 10  | PRO  |
| 13  | AM    | 63  | THR  |
| 13  | AM    | 67  | GLU  |
| 13  | AM    | 117 | VAL  |
| 14  | AN    | 14  | PRO  |
| 14  | AN    | 16  | PHE  |
| 14  | AN    | 29  | ARG  |
| 14  | AN    | 59  | ALA  |
| 15  | AO    | 24  | SER  |
| 18  | AR    | 87  | ARG  |
| 19  | AS    | 63  | THR  |
| 24  | AY    | 40  | HIS  |
| 24  | AY    | 57  | GLN  |
| 24  | AY    | 82  | ILE  |
| 24  | AY    | 206 | LEU  |
| 24  | AY    | 394 | ALA  |
| 24  | AY    | 402 | ILE  |
| 24  | AY    | 403 | GLU  |
| 24  | AY    | 530 | VAL  |
| 24  | AY    | 555 | LEU  |
| 25  | B0    | 37  | LEU  |
| 25  | B0    | 57  | PHE  |
| 26  | B1    | 83  | GLU  |
| 27  | B2    | 17  | SER  |
| 27  | B2    | 43  | GLN  |
| 27  | B2    | 48  | HIS  |
| 27  | B2    | 70  | GLN  |
| 27  | B2    | 71  | ASN  |
| 29  | B4    | 7   | PRO  |
| 29  | B4    | 15  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | B4    | 16  | CYS  |
| 29  | B4    | 22  | ILE  |
| 29  | B4    | 24  | THR  |
| 29  | B4    | 25  | TYR  |
| 29  | B4    | 29  | PRO  |
| 29  | B4    | 33  | VAL  |
| 29  | B4    | 34  | GLU  |
| 29  | B4    | 35  | VAL  |
| 29  | B4    | 38  | LYS  |
| 29  | B4    | 40  | HIS  |
| 29  | B4    | 55  | ARG  |
| 29  | B4    | 60  | GLN  |
| 29  | B4    | 66  | SER  |
| 30  | B5    | 4   | HIS  |
| 30  | B5    | 48  | GLU  |
| 30  | B5    | 49  | CYS  |
| 30  | B5    | 52  | TYR  |
| 30  | B5    | 53  | ALA  |
| 30  | B5    | 54  | GLY  |
| 30  | B5    | 57  | VAL  |
| 31  | B6    | 18  | ARG  |
| 31  | B6    | 20  | ASN  |
| 31  | B6    | 27  | LYS  |
| 31  | B6    | 31  | PRO  |
| 31  | B6    | 33  | LYS  |
| 31  | B6    | 46  | HIS  |
| 31  | B6    | 52  | VAL  |
| 33  | B8    | 29  | LYS  |
| 33  | B8    | 33  | ASN  |
| 33  | B8    | 34  | TRP  |
| 33  | B8    | 35  | GLN  |
| 33  | B8    | 61  | LEU  |
| 33  | B8    | 64  | TYR  |
| 37  | BC    | 42  | VAL  |
| 37  | BC    | 47  | LYS  |
| 37  | BC    | 68  | GLY  |
| 37  | BC    | 95  | VAL  |
| 37  | BC    | 101 | ILE  |
| 37  | BC    | 104 | ILE  |
| 37  | BC    | 117 | THR  |
| 37  | BC    | 145 | THR  |
| 37  | BC    | 148 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | BC    | 180 | SER  |
| 37  | BC    | 181 | PHE  |
| 38  | BD    | 24  | ILE  |
| 38  | BD    | 45  | ASN  |
| 38  | BD    | 125 | ILE  |
| 38  | BD    | 127 | VAL  |
| 38  | BD    | 267 | SER  |
| 39  | BE    | 2   | LYS  |
| 39  | BE    | 55  | ASN  |
| 39  | BE    | 56  | PRO  |
| 39  | BE    | 72  | VAL  |
| 39  | BE    | 76  | ARG  |
| 39  | BE    | 77  | ILE  |
| 39  | BE    | 88  | GLY  |
| 39  | BE    | 130 | GLY  |
| 39  | BE    | 155 | LYS  |
| 40  | BF    | 3   | GLU  |
| 40  | BF    | 11  | VAL  |
| 40  | BF    | 14  | PRO  |
| 40  | BF    | 21  | ALA  |
| 40  | BF    | 26  | ALA  |
| 40  | BF    | 82  | ILE  |
| 40  | BF    | 83  | PHE  |
| 40  | BF    | 89  | VAL  |
| 40  | BF    | 168 | ARG  |
| 41  | BG    | 8   | LYS  |
| 41  | BG    | 21  | ARG  |
| 41  | BG    | 22  | ARG  |
| 41  | BG    | 23  | PHE  |
| 41  | BG    | 25  | TYR  |
| 41  | BG    | 44  | GLY  |
| 41  | BG    | 48  | GLU  |
| 41  | BG    | 49  | ASP  |
| 41  | BG    | 54  | GLU  |
| 41  | BG    | 66  | GLN  |
| 41  | BG    | 73  | ALA  |
| 41  | BG    | 86  | MET  |
| 41  | BG    | 87  | PRO  |
| 41  | BG    | 88  | ILE  |
| 41  | BG    | 104 | GLU  |
| 41  | BG    | 109 | VAL  |
| 41  | BG    | 117 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BG    | 118 | ARG  |
| 41  | BG    | 122 | PRO  |
| 41  | BG    | 123 | ASN  |
| 41  | BG    | 143 | GLU  |
| 41  | BG    | 146 | TYR  |
| 41  | BG    | 181 | ARG  |
| 42  | BH    | 21  | PRO  |
| 42  | BH    | 55  | PRO  |
| 42  | BH    | 83  | TYR  |
| 42  | BH    | 126 | PRO  |
| 42  | BH    | 137 | ASP  |
| 42  | BH    | 138 | LYS  |
| 42  | BH    | 157 | TYR  |
| 42  | BH    | 167 | GLU  |
| 46  | BN    | 58  | ASP  |
| 46  | BN    | 127 | ASP  |
| 46  | BN    | 134 | ARG  |
| 48  | BP    | 10  | PRO  |
| 48  | BP    | 13  | ASN  |
| 48  | BP    | 15  | ARG  |
| 48  | BP    | 17  | LYS  |
| 48  | BP    | 19  | VAL  |
| 48  | BP    | 34  | GLY  |
| 48  | BP    | 39  | LYS  |
| 48  | BP    | 40  | SER  |
| 48  | BP    | 47  | ASP  |
| 48  | BP    | 58  | THR  |
| 48  | BP    | 61  | ARG  |
| 48  | BP    | 65  | ARG  |
| 48  | BP    | 103 | ALA  |
| 48  | BP    | 107 | LYS  |
| 48  | BP    | 108 | LYS  |
| 48  | BP    | 115 | LEU  |
| 48  | BP    | 140 | ALA  |
| 48  | BP    | 146 | VAL  |
| 49  | BQ    | 62  | GLY  |
| 50  | BR    | 4   | LEU  |
| 50  | BR    | 117 | VAL  |
| 51  | BS    | 53  | SER  |
| 51  | BS    | 88  | ASP  |
| 51  | BS    | 92  | TYR  |
| 51  | BS    | 93  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | BS    | 105 | ALA  |
| 52  | BT    | 23  | ARG  |
| 52  | BT    | 28  | VAL  |
| 52  | BT    | 30  | VAL  |
| 52  | BT    | 32  | TYR  |
| 52  | BT    | 33  | LYS  |
| 52  | BT    | 80  | SER  |
| 52  | BT    | 88  | ILE  |
| 52  | BT    | 91  | ARG  |
| 52  | BT    | 107 | ASP  |
| 52  | BT    | 119 | LYS  |
| 52  | BT    | 127 | ALA  |
| 53  | BU    | 89  | GLU  |
| 53  | BU    | 91  | ASP  |
| 54  | BV    | 2   | PHE  |
| 54  | BV    | 16  | PRO  |
| 54  | BV    | 53  | GLU  |
| 55  | BW    | 63  | ASP  |
| 57  | BY    | 17  | SER  |
| 57  | BY    | 27  | VAL  |
| 57  | BY    | 30  | VAL  |
| 57  | BY    | 50  | ARG  |
| 57  | BY    | 51  | VAL  |
| 57  | BY    | 56  | PRO  |
| 57  | BY    | 57  | GLN  |
| 57  | BY    | 62  | GLU  |
| 57  | BY    | 77  | PRO  |
| 57  | BY    | 78  | ALA  |
| 57  | BY    | 80  | GLY  |
| 57  | BY    | 90  | LEU  |
| 57  | BY    | 98  | VAL  |
| 57  | BY    | 99  | CYS  |
| 58  | BZ    | 31  | ARG  |
| 58  | BZ    | 61  | LEU  |
| 58  | BZ    | 113 | ALA  |
| 58  | BZ    | 124 | ILE  |
| 58  | BZ    | 152 | ALA  |
| 58  | BZ    | 186 | GLU  |
| 2   | AB    | 17  | PHE  |
| 2   | AB    | 28  | PHE  |
| 2   | AB    | 40  | HIS  |
| 2   | AB    | 91  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 95  | GLN  |
| 2   | AB    | 228 | GLY  |
| 3   | AC    | 13  | GLY  |
| 3   | AC    | 22  | TRP  |
| 3   | AC    | 26  | LYS  |
| 3   | AC    | 85  | ARG  |
| 3   | AC    | 168 | ALA  |
| 3   | AC    | 181 | ASN  |
| 3   | AC    | 207 | VAL  |
| 4   | AD    | 3   | ARG  |
| 4   | AD    | 26  | CYS  |
| 4   | AD    | 30  | LYS  |
| 4   | AD    | 88  | VAL  |
| 4   | AD    | 110 | PHE  |
| 6   | AF    | 39  | LYS  |
| 6   | AF    | 40  | VAL  |
| 9   | AI    | 11  | LYS  |
| 9   | AI    | 41  | VAL  |
| 9   | AI    | 127 | LYS  |
| 10  | AJ    | 32  | ALA  |
| 10  | AJ    | 86  | MET  |
| 12  | AL    | 79  | GLU  |
| 13  | AM    | 4   | ILE  |
| 13  | AM    | 12  | ASN  |
| 13  | AM    | 28  | ALA  |
| 13  | AM    | 46  | LYS  |
| 14  | AN    | 24  | CYS  |
| 16  | AP    | 83  | GLU  |
| 17  | AQ    | 33  | GLY  |
| 19  | AS    | 27  | GLU  |
| 19  | AS    | 62  | ILE  |
| 19  | AS    | 64  | GLU  |
| 20  | AT    | 101 | GLY  |
| 21  | AU    | 3   | LYS  |
| 21  | AU    | 25  | LYS  |
| 24  | AY    | 6   | GLU  |
| 24  | AY    | 25  | LYS  |
| 24  | AY    | 45  | VAL  |
| 24  | AY    | 58  | GLU  |
| 24  | AY    | 110 | SER  |
| 24  | AY    | 114 | VAL  |
| 24  | AY    | 197 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | AY    | 224 | ASP  |
| 24  | AY    | 400 | GLU  |
| 24  | AY    | 401 | SER  |
| 24  | AY    | 447 | GLY  |
| 24  | AY    | 536 | LYS  |
| 25  | B0    | 5   | LYS  |
| 25  | B0    | 8   | GLY  |
| 25  | B0    | 11  | ARG  |
| 25  | B0    | 12  | ASN  |
| 25  | B0    | 79  | VAL  |
| 26  | B1    | 7   | ILE  |
| 26  | B1    | 53  | VAL  |
| 27  | B2    | 10  | LEU  |
| 27  | B2    | 36  | ARG  |
| 27  | B2    | 47  | ASN  |
| 29  | B4    | 20  | ASN  |
| 29  | B4    | 31  | ILE  |
| 29  | B4    | 39  | CYS  |
| 29  | B4    | 44  | THR  |
| 29  | B4    | 48  | ARG  |
| 29  | B4    | 49  | PHE  |
| 29  | B4    | 52  | THR  |
| 29  | B4    | 56  | VAL  |
| 29  | B4    | 61  | ARG  |
| 29  | B4    | 65  | ASP  |
| 30  | B5    | 55  | ARG  |
| 31  | B6    | 28  | ARG  |
| 31  | B6    | 29  | ASN  |
| 31  | B6    | 44  | ARG  |
| 31  | B6    | 51  | GLU  |
| 34  | B9    | 36  | GLN  |
| 37  | BC    | 53  | ARG  |
| 37  | BC    | 81  | GLY  |
| 37  | BC    | 85  | LYS  |
| 37  | BC    | 92  | ALA  |
| 37  | BC    | 99  | GLU  |
| 37  | BC    | 102 | GLN  |
| 37  | BC    | 105 | LEU  |
| 37  | BC    | 106 | ASP  |
| 37  | BC    | 109 | MET  |
| 37  | BC    | 130 | ARG  |
| 37  | BC    | 143 | ALA  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 37         | BC           | 150        | ILE         |
| 37         | BC           | 159        | ALA         |
| 37         | BC           | 161        | ARG         |
| 37         | BC           | 179        | ALA         |
| 38         | BD           | 28         | GLU         |
| 38         | BD           | 239        | ARG         |
| 38         | BD           | 242        | ARG         |
| 38         | BD           | 244        | ARG         |
| 38         | BD           | 268        | ARG         |
| 39         | BE           | 71         | GLY         |
| 39         | BE           | 75         | VAL         |
| 39         | BE           | 121        | ASN         |
| 39         | BE           | 186        | GLY         |
| 40         | BF           | 5          | ALA         |
| 40         | BF           | 25         | PRO         |
| 40         | BF           | 78         | ILE         |
| 40         | BF           | 134        | GLY         |
| 40         | BF           | 167        | ALA         |
| 41         | BG           | 6          | ALA         |
| 41         | BG           | 24         | GLY         |
| 41         | BG           | 43         | LEU         |
| 41         | BG           | 52         | ILE         |
| 41         | BG           | 78         | SER         |
| 41         | BG           | 97         | ASP         |
| 41         | BG           | 98         | ARG         |
| 41         | BG           | 115        | ARG         |
| 41         | BG           | 128        | ARG         |
| 41         | BG           | 129        | GLY         |
| 41         | BG           | 132        | ASN         |
| 41         | BG           | 138        | GLN         |
| 41         | BG           | 162        | THR         |
| 41         | BG           | 163        | ALA         |
| 42         | BH           | 2          | SER         |
| 42         | BH           | 14         | GLY         |
| 42         | BH           | 66         | GLY         |
| 42         | BH           | 156        | ALA         |
| 42         | BH           | 158        | HIS         |
| 46         | BN           | 19         | GLU         |
| 46         | BN           | 57         | ALA         |
| 47         | BO           | 5          | GLN         |
| 47         | BO           | 49         | ARG         |
| 47         | BO           | 111        | PHE         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | BP    | 12  | ALA  |
| 48  | BP    | 26  | GLY  |
| 48  | BP    | 76  | LYS  |
| 48  | BP    | 109 | GLY  |
| 48  | BP    | 116 | GLY  |
| 48  | BP    | 117 | GLU  |
| 48  | BP    | 147 | LEU  |
| 49  | BQ    | 60  | ARG  |
| 50  | BR    | 10  | LEU  |
| 50  | BR    | 86  | ARG  |
| 51  | BS    | 58  | LEU  |
| 51  | BS    | 62  | LYS  |
| 51  | BS    | 90  | GLY  |
| 51  | BS    | 94  | TYR  |
| 51  | BS    | 97  | ARG  |
| 51  | BS    | 103 | GLU  |
| 52  | BT    | 29  | ARG  |
| 52  | BT    | 78  | LEU  |
| 53  | BU    | 88  | ILE  |
| 54  | BV    | 23  | GLU  |
| 54  | BV    | 40  | LEU  |
| 54  | BV    | 46  | VAL  |
| 54  | BV    | 47  | VAL  |
| 54  | BV    | 50  | PRO  |
| 54  | BV    | 67  | GLY  |
| 55  | BW    | 11  | ARG  |
| 55  | BW    | 68  | ARG  |
| 57  | BY    | 42  | VAL  |
| 58  | BZ    | 30  | ASN  |
| 58  | BZ    | 81  | ARG  |
| 58  | BZ    | 147 | GLY  |
| 58  | BZ    | 148 | ASP  |
| 58  | BZ    | 150 | LEU  |
| 2   | AB    | 75  | LYS  |
| 2   | AB    | 92  | TYR  |
| 2   | AB    | 125 | PRO  |
| 2   | AB    | 157 | ARG  |
| 3   | AC    | 54  | ARG  |
| 4   | AD    | 37  | PRO  |
| 4   | AD    | 189 | PRO  |
| 5   | AE    | 70  | PRO  |
| 6   | AF    | 13  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | AG    | 57  | GLU  |
| 7   | AG    | 89  | MET  |
| 8   | AH    | 2   | LEU  |
| 10  | AJ    | 29  | ARG  |
| 10  | AJ    | 30  | SER  |
| 10  | AJ    | 59  | SER  |
| 13  | AM    | 51  | ALA  |
| 17  | AQ    | 68  | ARG  |
| 18  | AR    | 54  | ARG  |
| 19  | AS    | 8   | GLY  |
| 19  | AS    | 9   | VAL  |
| 19  | AS    | 85  | LYS  |
| 20  | AT    | 73  | HIS  |
| 20  | AT    | 95  | ALA  |
| 24  | AY    | 22  | ASP  |
| 24  | AY    | 55  | MET  |
| 24  | AY    | 127 | LYS  |
| 24  | AY    | 171 | GLU  |
| 24  | AY    | 204 | GLU  |
| 24  | AY    | 297 | GLU  |
| 29  | B4    | 36  | CYS  |
| 29  | B4    | 51  | ASP  |
| 31  | B6    | 9   | LEU  |
| 31  | B6    | 16  | CYS  |
| 31  | B6    | 45  | LYS  |
| 33  | B8    | 31  | HIS  |
| 33  | B8    | 49  | VAL  |
| 34  | B9    | 10  | ILE  |
| 37  | BC    | 30  | VAL  |
| 37  | BC    | 43  | GLU  |
| 37  | BC    | 52  | PRO  |
| 37  | BC    | 69  | LEU  |
| 37  | BC    | 107 | GLY  |
| 37  | BC    | 119 | ASP  |
| 37  | BC    | 128 | LEU  |
| 37  | BC    | 134 | PRO  |
| 37  | BC    | 184 | GLU  |
| 37  | BC    | 202 | PRO  |
| 37  | BC    | 209 | PHE  |
| 38  | BD    | 35  | LYS  |
| 38  | BD    | 262 | ARG  |
| 38  | BD    | 263 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BE    | 53  | PRO  |
| 39  | BE    | 54  | GLN  |
| 39  | BE    | 70  | ALA  |
| 39  | BE    | 82  | ARG  |
| 39  | BE    | 187 | ALA  |
| 40  | BF    | 10  | PRO  |
| 40  | BF    | 84  | VAL  |
| 40  | BF    | 135 | LYS  |
| 41  | BG    | 133 | LEU  |
| 41  | BG    | 137 | GLU  |
| 41  | BG    | 155 | MET  |
| 42  | BH    | 12  | PRO  |
| 42  | BH    | 24  | VAL  |
| 42  | BH    | 81  | GLU  |
| 42  | BH    | 154 | PRO  |
| 42  | BH    | 170 | ARG  |
| 48  | BP    | 49  | ARG  |
| 48  | BP    | 106 | LEU  |
| 48  | BP    | 111 | ARG  |
| 48  | BP    | 149 | GLU  |
| 49  | BQ    | 13  | GLN  |
| 49  | BQ    | 115 | MET  |
| 50  | BR    | 88  | ARG  |
| 50  | BR    | 106 | GLY  |
| 51  | BS    | 13  | ARG  |
| 51  | BS    | 24  | LEU  |
| 51  | BS    | 51  | ALA  |
| 51  | BS    | 57  | LYS  |
| 52  | BT    | 118 | ARG  |
| 52  | BT    | 134 | GLU  |
| 52  | BT    | 136 | GLN  |
| 53  | BU    | 93  | LYS  |
| 54  | BV    | 19  | LYS  |
| 55  | BW    | 6   | ILE  |
| 57  | BY    | 39  | VAL  |
| 57  | BY    | 40  | GLU  |
| 57  | BY    | 53  | PRO  |
| 57  | BY    | 100 | ALA  |
| 58  | BZ    | 12  | GLY  |
| 58  | BZ    | 22  | GLY  |
| 58  | BZ    | 80  | ARG  |
| 58  | BZ    | 128 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 190 | THR  |
| 3   | AC    | 4   | LYS  |
| 3   | AC    | 29  | TYR  |
| 3   | AC    | 61  | ALA  |
| 3   | AC    | 80  | GLY  |
| 3   | AC    | 170 | GLN  |
| 5   | AE    | 8   | GLU  |
| 6   | AF    | 16  | GLN  |
| 12  | AL    | 115 | LYS  |
| 13  | AM    | 85  | GLY  |
| 14  | AN    | 56  | VAL  |
| 14  | AN    | 60  | SER  |
| 16  | AP    | 53  | VAL  |
| 19  | AS    | 18  | LYS  |
| 19  | AS    | 89  | ALA  |
| 19  | AS    | 90  | THR  |
| 20  | AT    | 71  | THR  |
| 20  | AT    | 74  | LYS  |
| 20  | AT    | 97  | ALA  |
| 24  | AY    | 49  | ALA  |
| 24  | AY    | 551 | GLN  |
| 27  | B2    | 35  | LEU  |
| 27  | B2    | 46  | GLN  |
| 27  | B2    | 50  | ILE  |
| 29  | B4    | 21  | VAL  |
| 29  | B4    | 42  | PHE  |
| 29  | B4    | 47  | GLN  |
| 29  | B4    | 59  | PHE  |
| 29  | B4    | 67  | TYR  |
| 30  | B5    | 51  | TYR  |
| 31  | B6    | 23  | THR  |
| 33  | B8    | 3   | LYS  |
| 37  | BC    | 16  | ASP  |
| 37  | BC    | 88  | GLU  |
| 37  | BC    | 141 | PRO  |
| 37  | BC    | 142 | LYS  |
| 38  | BD    | 3   | VAL  |
| 38  | BD    | 241 | PRO  |
| 39  | BE    | 69  | LYS  |
| 40  | BF    | 81  | PRO  |
| 41  | BG    | 26  | GLN  |
| 41  | BG    | 46  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BG    | 57  | ALA  |
| 42  | BH    | 160 | LYS  |
| 46  | BN    | 8   | GLN  |
| 46  | BN    | 59  | LYS  |
| 46  | BN    | 68  | GLU  |
| 48  | BP    | 9   | ASN  |
| 48  | BP    | 25  | SER  |
| 48  | BP    | 33  | ARG  |
| 49  | BQ    | 20  | ALA  |
| 49  | BQ    | 140 | ALA  |
| 51  | BS    | 14  | VAL  |
| 51  | BS    | 102 | ALA  |
| 52  | BT    | 3   | ARG  |
| 52  | BT    | 12  | SER  |
| 53  | BU    | 50  | ARG  |
| 56  | BX    | 13  | LEU  |
| 57  | BY    | 97  | ARG  |
| 58  | BZ    | 14  | LYS  |
| 58  | BZ    | 78  | LYS  |
| 2   | AB    | 8   | LYS  |
| 2   | AB    | 16  | HIS  |
| 3   | AC    | 32  | LEU  |
| 3   | AC    | 66  | VAL  |
| 3   | AC    | 118 | GLN  |
| 3   | AC    | 121 | ALA  |
| 3   | AC    | 187 | ALA  |
| 4   | AD    | 191 | ARG  |
| 6   | AF    | 70  | ASP  |
| 7   | AG    | 4   | ARG  |
| 7   | AG    | 47  | CYS  |
| 7   | AG    | 58  | PRO  |
| 7   | AG    | 128 | ALA  |
| 9   | AI    | 54  | ASP  |
| 10  | AJ    | 18  | ALA  |
| 12  | AL    | 29  | GLY  |
| 12  | AL    | 45  | PRO  |
| 12  | AL    | 95  | GLY  |
| 19  | AS    | 41  | VAL  |
| 19  | AS    | 87  | ALA  |
| 20  | AT    | 100 | ILE  |
| 24  | AY    | 47  | GLU  |
| 24  | AY    | 59  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | AY    | 183 | MET  |
| 24  | AY    | 205 | TYR  |
| 24  | AY    | 210 | ARG  |
| 24  | AY    | 253 | LEU  |
| 24  | AY    | 380 | LEU  |
| 24  | AY    | 506 | GLN  |
| 24  | AY    | 574 | GLU  |
| 27  | B2    | 5   | GLU  |
| 27  | B2    | 16  | LEU  |
| 28  | B3    | 16  | PRO  |
| 29  | B4    | 2   | LYS  |
| 29  | B4    | 6   | HIS  |
| 29  | B4    | 9   | LEU  |
| 33  | B8    | 32  | LEU  |
| 33  | B8    | 43  | GLN  |
| 34  | B9    | 11  | CYS  |
| 37  | BC    | 21  | TYR  |
| 37  | BC    | 89  | GLU  |
| 37  | BC    | 116 | ALA  |
| 37  | BC    | 126 | SER  |
| 39  | BE    | 52  | LEU  |
| 40  | BF    | 9   | ILE  |
| 41  | BG    | 93  | THR  |
| 42  | BH    | 13  | LYS  |
| 42  | BH    | 19  | VAL  |
| 42  | BH    | 40  | GLU  |
| 42  | BH    | 85  | LYS  |
| 42  | BH    | 98  | LEU  |
| 42  | BH    | 159 | GLU  |
| 42  | BH    | 168 | PRO  |
| 46  | BN    | 5   | VAL  |
| 48  | BP    | 67  | MET  |
| 48  | BP    | 141 | ALA  |
| 50  | BR    | 8   | ARG  |
| 50  | BR    | 11  | ASN  |
| 52  | BT    | 7   | ILE  |
| 52  | BT    | 17  | THR  |
| 54  | BV    | 44  | LYS  |
| 54  | BV    | 48  | GLY  |
| 57  | BY    | 3   | VAL  |
| 57  | BY    | 10  | GLY  |
| 57  | BY    | 31  | LEU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 57         | BY           | 61         | ILE         |
| 58         | BZ           | 63         | ASP         |
| 58         | BZ           | 158        | PRO         |
| 58         | BZ           | 162        | GLU         |
| 58         | BZ           | 183        | LEU         |
| 2          | AB           | 130        | ARG         |
| 2          | AB           | 158        | LEU         |
| 3          | AC           | 65         | ALA         |
| 4          | AD           | 150        | GLU         |
| 4          | AD           | 171        | GLY         |
| 5          | AE           | 22         | GLY         |
| 7          | AG           | 20         | ASP         |
| 9          | AI           | 89         | ASN         |
| 11         | AK           | 117        | ASN         |
| 24         | AY           | 23         | ALA         |
| 24         | AY           | 60         | GLU         |
| 24         | AY           | 81         | ILE         |
| 24         | AY           | 230        | LYS         |
| 24         | AY           | 239        | GLU         |
| 24         | AY           | 531        | GLY         |
| 24         | AY           | 554        | PRO         |
| 24         | AY           | 577        | SER         |
| 24         | AY           | 680        | PRO         |
| 37         | BC           | 221        | PRO         |
| 38         | BD           | 36         | PRO         |
| 39         | BE           | 45         | THR         |
| 39         | BE           | 73         | GLU         |
| 40         | BF           | 204        | ASN         |
| 41         | BG           | 30         | GLU         |
| 41         | BG           | 50         | ALA         |
| 41         | BG           | 94         | LEU         |
| 41         | BG           | 165        | THR         |
| 42         | BH           | 9          | ILE         |
| 46         | BN           | 125        | GLY         |
| 46         | BN           | 129        | PRO         |
| 48         | BP           | 43         | GLY         |
| 52         | BT           | 31         | SER         |
| 57         | BY           | 4          | LYS         |
| 57         | BY           | 81         | LYS         |
| 57         | BY           | 88         | LYS         |
| 2          | AB           | 234        | PRO         |
| 2          | AB           | 239        | VAL         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 130 | VAL  |
| 10  | AJ    | 4   | ILE  |
| 20  | AT    | 102 | GLY  |
| 24  | AY    | 37  | GLY  |
| 24  | AY    | 404 | VAL  |
| 26  | B1    | 30  | VAL  |
| 38  | BD    | 238 | GLY  |
| 40  | BF    | 30  | PRO  |
| 46  | BN    | 40  | PRO  |
| 48  | BP    | 144 | GLU  |
| 51  | BS    | 82  | ILE  |
| 54  | BV    | 35  | LEU  |
| 57  | BY    | 52  | SER  |
| 26  | B1    | 86  | SER  |
| 29  | B4    | 41  | PRO  |
| 37  | BC    | 75  | VAL  |
| 37  | BC    | 84  | ILE  |
| 39  | BE    | 175 | VAL  |
| 40  | BF    | 6   | VAL  |
| 41  | BG    | 141 | PHE  |
| 41  | BG    | 142 | PRO  |
| 42  | BH    | 111 | HIS  |
| 53  | BU    | 90  | VAL  |
| 7   | AG    | 17  | VAL  |
| 9   | AI    | 81  | ILE  |
| 12  | AL    | 48  | PRO  |
| 33  | B8    | 63  | PRO  |
| 48  | BP    | 11  | GLY  |
| 51  | BS    | 60  | GLY  |
| 54  | BV    | 79  | VAL  |
| 39  | BE    | 62  | PRO  |
| 42  | BH    | 92  | ILE  |
| 51  | BS    | 98  | VAL  |
| 54  | BV    | 52  | VAL  |
| 58  | BZ    | 176 | PRO  |
| 11  | AK    | 49  | GLY  |
| 12  | AL    | 18  | VAL  |
| 13  | AM    | 24  | GLY  |
| 42  | BH    | 20  | ALA  |
| 42  | BH    | 10  | PRO  |
| 38  | 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%)  | 157 (78%) | 45 (22%) | 1           | 4  |
| 3   | AC    | 160/188 (85%)  | 129 (81%) | 31 (19%) | 1           | 7  |
| 4   | AD    | 180/181 (99%)  | 155 (86%) | 25 (14%) | 4           | 16 |
| 5   | AE    | 115/123 (94%)  | 109 (95%) | 6 (5%)   | 27          | 63 |
| 6   | AF    | 90/90 (100%)   | 83 (92%)  | 7 (8%)   | 15          | 44 |
| 7   | AG    | 126/127 (99%)  | 108 (86%) | 18 (14%) | 4           | 16 |
| 8   | AH    | 119/119 (100%) | 103 (87%) | 16 (13%) | 4           | 18 |
| 9   | AI    | 98/99 (99%)    | 85 (87%)  | 13 (13%) | 4           | 18 |
| 10  | AJ    | 88/92 (96%)    | 82 (93%)  | 6 (7%)   | 18          | 51 |
| 11  | AK    | 90/99 (91%)    | 84 (93%)  | 6 (7%)   | 19          | 52 |
| 12  | AL    | 104/109 (95%)  | 90 (86%)  | 14 (14%) | 4           | 17 |
| 13  | AM    | 94/101 (93%)   | 84 (89%)  | 10 (11%) | 8           | 28 |
| 14  | AN    | 49/50 (98%)    | 43 (88%)  | 6 (12%)  | 6           | 22 |
| 15  | AO    | 79/80 (99%)    | 71 (90%)  | 8 (10%)  | 9           | 30 |
| 16  | AP    | 72/74 (97%)    | 68 (94%)  | 4 (6%)   | 25          | 60 |
| 17  | AQ    | 94/97 (97%)    | 92 (98%)  | 2 (2%)   | 59          | 85 |
| 18  | AR    | 61/77 (79%)    | 55 (90%)  | 6 (10%)  | 9           | 32 |
| 19  | AS    | 74/80 (92%)    | 68 (92%)  | 6 (8%)   | 14          | 42 |
| 20  | AT    | 76/82 (93%)    | 68 (90%)  | 8 (10%)  | 8           | 28 |
| 21  | AU    | 19/22 (86%)    | 18 (95%)  | 1 (5%)   | 26          | 62 |
| 24  | AY    | 579/582 (100%) | 516 (89%) | 63 (11%) | 7           | 26 |
| 25  | B0    | 66/66 (100%)   | 45 (68%)  | 21 (32%) | 0           | 1  |
| 26  | B1    | 78/82 (95%)    | 60 (77%)  | 18 (23%) | 1           | 4  |
| 27  | B2    | 66/66 (100%)   | 42 (64%)  | 24 (36%) | 0           | 1  |
| 28  | B3    | 51/52 (98%)    | 44 (86%)  | 7 (14%)  | 4           | 17 |
| 29  | B4    | 63/63 (100%)   | 48 (76%)  | 15 (24%) | 1           | 3  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |     |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 30  | B5    | 51/51 (100%)    | 42 (82%)   | 9 (18%)   | 2           | 9   |
| 31  | B6    | 49/51 (96%)     | 37 (76%)   | 12 (24%)  | 1           | 3   |
| 32  | B7    | 41/41 (100%)    | 39 (95%)   | 2 (5%)    | 29          | 65  |
| 33  | B8    | 53/54 (98%)     | 42 (79%)   | 11 (21%)  | 1           | 5   |
| 34  | B9    | 34/34 (100%)    | 31 (91%)   | 3 (9%)    | 12          | 38  |
| 37  | BC    | 179/180 (99%)   | 160 (89%)  | 19 (11%)  | 8           | 28  |
| 38  | BD    | 217/217 (100%)  | 185 (85%)  | 32 (15%)  | 3           | 14  |
| 39  | BE    | 165/166 (99%)   | 133 (81%)  | 32 (19%)  | 1           | 7   |
| 40  | BF    | 165/166 (99%)   | 146 (88%)  | 19 (12%)  | 6           | 24  |
| 41  | BG    | 153/155 (99%)   | 123 (80%)  | 30 (20%)  | 1           | 7   |
| 42  | BH    | 146/148 (99%)   | 131 (90%)  | 15 (10%)  | 8           | 29  |
| 43  | BJ    | 1/1 (100%)      | 1 (100%)   | 0         | 100         | 100 |
| 46  | BN    | 117/119 (98%)   | 103 (88%)  | 14 (12%)  | 6           | 23  |
| 47  | BO    | 100/100 (100%)  | 93 (93%)   | 7 (7%)    | 18          | 50  |
| 48  | BP    | 112/115 (97%)   | 84 (75%)   | 28 (25%)  | 1           | 2   |
| 49  | BQ    | 111/111 (100%)  | 96 (86%)   | 15 (14%)  | 4           | 17  |
| 50  | BR    | 100/100 (100%)  | 82 (82%)   | 18 (18%)  | 2           | 9   |
| 51  | BS    | 77/87 (88%)     | 62 (80%)   | 15 (20%)  | 1           | 7   |
| 52  | BT    | 120/127 (94%)   | 94 (78%)   | 26 (22%)  | 1           | 5   |
| 53  | BU    | 92/93 (99%)     | 80 (87%)   | 12 (13%)  | 5           | 19  |
| 54  | BV    | 82/82 (100%)    | 65 (79%)   | 17 (21%)  | 1           | 5   |
| 55  | BW    | 91/92 (99%)     | 79 (87%)   | 12 (13%)  | 5           | 18  |
| 56  | BX    | 74/77 (96%)     | 68 (92%)   | 6 (8%)    | 14          | 42  |
| 57  | BY    | 84/90 (93%)     | 65 (77%)   | 19 (23%)  | 1           | 4   |
| 58  | BZ    | 162/178 (91%)   | 138 (85%)  | 24 (15%)  | 3           | 14  |
| All | All   | 5469/5656 (97%) | 4686 (86%) | 783 (14%) | 4           | 16  |

All (783) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 16  | HIS  |
| 2   | AB    | 17  | PHE  |
| 2   | AB    | 22  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 23  | ARG  |
| 2   | AB    | 24  | TRP  |
| 2   | AB    | 28  | PHE  |
| 2   | AB    | 36  | ARG  |
| 2   | AB    | 42  | ILE  |
| 2   | AB    | 48  | MET  |
| 2   | AB    | 52  | GLU  |
| 2   | AB    | 60  | ASP  |
| 2   | AB    | 74  | LYS  |
| 2   | AB    | 76  | GLN  |
| 2   | AB    | 82  | ARG  |
| 2   | AB    | 83  | MET  |
| 2   | AB    | 87  | ARG  |
| 2   | AB    | 90  | MET  |
| 2   | AB    | 93  | VAL  |
| 2   | AB    | 96  | ARG  |
| 2   | AB    | 101 | MET  |
| 2   | AB    | 102 | LEU  |
| 2   | AB    | 109 | SER  |
| 2   | AB    | 110 | GLN  |
| 2   | AB    | 114 | ARG  |
| 2   | AB    | 116 | GLU  |
| 2   | AB    | 122 | PHE  |
| 2   | AB    | 127 | ILE  |
| 2   | AB    | 137 | ARG  |
| 2   | AB    | 142 | LEU  |
| 2   | AB    | 149 | LEU  |
| 2   | AB    | 153 | ARG  |
| 2   | AB    | 157 | ARG  |
| 2   | AB    | 163 | PHE  |
| 2   | AB    | 170 | GLU  |
| 2   | AB    | 178 | ARG  |
| 2   | AB    | 185 | ILE  |
| 2   | AB    | 187 | LEU  |
| 2   | AB    | 191 | ASP  |
| 2   | AB    | 198 | ASP  |
| 2   | AB    | 200 | ILE  |
| 2   | AB    | 204 | ASN  |
| 2   | AB    | 224 | GLN  |
| 2   | AB    | 229 | VAL  |
| 2   | AB    | 231 | GLU  |
| 2   | AB    | 233 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 3   | ASN  |
| 3   | AC    | 5   | ILE  |
| 3   | AC    | 14  | ILE  |
| 3   | AC    | 16  | ARG  |
| 3   | AC    | 20  | SER  |
| 3   | AC    | 21  | ARG  |
| 3   | AC    | 26  | LYS  |
| 3   | AC    | 30  | ARG  |
| 3   | AC    | 34  | LEU  |
| 3   | AC    | 46  | GLU  |
| 3   | AC    | 52  | LEU  |
| 3   | AC    | 54  | ARG  |
| 3   | AC    | 63  | ASN  |
| 3   | AC    | 72  | LYS  |
| 3   | AC    | 76  | VAL  |
| 3   | AC    | 82  | GLU  |
| 3   | AC    | 86  | VAL  |
| 3   | AC    | 94  | LEU  |
| 3   | AC    | 101 | LEU  |
| 3   | AC    | 110 | ASN  |
| 3   | AC    | 111 | LEU  |
| 3   | AC    | 119 | ARG  |
| 3   | AC    | 123 | GLN  |
| 3   | AC    | 131 | ARG  |
| 3   | AC    | 132 | ARG  |
| 3   | AC    | 143 | GLU  |
| 3   | AC    | 164 | ARG  |
| 3   | AC    | 165 | THR  |
| 3   | AC    | 166 | GLU  |
| 3   | AC    | 167 | TRP  |
| 3   | AC    | 178 | LEU  |
| 4   | AD    | 3   | ARG  |
| 4   | AD    | 8   | VAL  |
| 4   | AD    | 13  | ARG  |
| 4   | AD    | 15  | GLU  |
| 4   | AD    | 21  | LEU  |
| 4   | AD    | 34  | GLU  |
| 4   | AD    | 36  | ARG  |
| 4   | AD    | 50  | ARG  |
| 4   | AD    | 58  | LEU  |
| 4   | AD    | 76  | ARG  |
| 4   | AD    | 88  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AD    | 101 | LEU  |
| 4   | AD    | 110 | PHE  |
| 4   | AD    | 112 | VAL  |
| 4   | AD    | 127 | THR  |
| 4   | AD    | 131 | ARG  |
| 4   | AD    | 132 | ARG  |
| 4   | AD    | 135 | LEU  |
| 4   | AD    | 139 | ARG  |
| 4   | AD    | 168 | ARG  |
| 4   | AD    | 190 | ASP  |
| 4   | AD    | 194 | LEU  |
| 4   | AD    | 196 | LEU  |
| 4   | AD    | 200 | GLU  |
| 4   | AD    | 209 | ARG  |
| 5   | AE    | 10  | MET  |
| 5   | AE    | 20  | GLN  |
| 5   | AE    | 31  | LEU  |
| 5   | AE    | 68  | GLU  |
| 5   | AE    | 73  | ASN  |
| 5   | AE    | 91  | LEU  |
| 6   | AF    | 19  | LEU  |
| 6   | AF    | 25  | ILE  |
| 6   | AF    | 32  | ASN  |
| 6   | AF    | 43  | LEU  |
| 6   | AF    | 67  | MET  |
| 6   | AF    | 69  | GLU  |
| 6   | AF    | 73  | ASN  |
| 7   | AG    | 22  | LEU  |
| 7   | AG    | 32  | ARG  |
| 7   | AG    | 33  | ASP  |
| 7   | AG    | 35  | LYS  |
| 7   | AG    | 38  | LEU  |
| 7   | AG    | 57  | GLU  |
| 7   | AG    | 78  | ARG  |
| 7   | AG    | 79  | ARG  |
| 7   | AG    | 90  | GLU  |
| 7   | AG    | 94  | ARG  |
| 7   | AG    | 104 | LEU  |
| 7   | AG    | 106 | GLN  |
| 7   | AG    | 114 | ARG  |
| 7   | AG    | 119 | ARG  |
| 7   | AG    | 131 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | AG    | 136 | LYS  |
| 7   | AG    | 140 | ASP  |
| 7   | AG    | 154 | TYR  |
| 8   | AH    | 1   | MET  |
| 8   | AH    | 6   | ILE  |
| 8   | AH    | 26  | VAL  |
| 8   | AH    | 27  | PRO  |
| 8   | AH    | 30  | ARG  |
| 8   | AH    | 39  | LEU  |
| 8   | AH    | 52  | ASP  |
| 8   | AH    | 54  | ASP  |
| 8   | AH    | 56  | LYS  |
| 8   | AH    | 63  | LEU  |
| 8   | AH    | 91  | ARG  |
| 8   | AH    | 92  | ARG  |
| 8   | AH    | 102 | ARG  |
| 8   | AH    | 105 | ARG  |
| 8   | AH    | 112 | LEU  |
| 8   | AH    | 127 | LEU  |
| 9   | AI    | 2   | GLU  |
| 9   | AI    | 14  | VAL  |
| 9   | AI    | 19  | LEU  |
| 9   | AI    | 20  | ARG  |
| 9   | AI    | 23  | ASN  |
| 9   | AI    | 26  | VAL  |
| 9   | AI    | 53  | VAL  |
| 9   | AI    | 60  | ASP  |
| 9   | AI    | 95  | LYS  |
| 9   | AI    | 104 | ARG  |
| 9   | AI    | 118 | LYS  |
| 9   | AI    | 121 | ARG  |
| 9   | AI    | 128 | ARG  |
| 10  | AJ    | 6   | ILE  |
| 10  | AJ    | 8   | LEU  |
| 10  | AJ    | 57  | LYS  |
| 10  | AJ    | 78  | ASN  |
| 10  | AJ    | 95  | GLU  |
| 10  | AJ    | 96  | ILE  |
| 11  | AK    | 53  | SER  |
| 11  | AK    | 81  | ASP  |
| 11  | AK    | 96  | ARG  |
| 11  | AK    | 104 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | AK    | 124 | LYS  |
| 11  | AK    | 126 | ARG  |
| 12  | AL    | 7   | ILE  |
| 12  | AL    | 8   | ASN  |
| 12  | AL    | 20  | LYS  |
| 12  | AL    | 27  | LEU  |
| 12  | AL    | 33  | ARG  |
| 12  | AL    | 41  | ARG  |
| 12  | AL    | 42  | THR  |
| 12  | AL    | 44  | THR  |
| 12  | AL    | 79  | GLU  |
| 12  | AL    | 84  | LEU  |
| 12  | AL    | 89  | ARG  |
| 12  | AL    | 94  | PRO  |
| 12  | AL    | 118 | SER  |
| 12  | AL    | 123 | LYS  |
| 13  | AM    | 7   | VAL  |
| 13  | AM    | 8   | GLU  |
| 13  | AM    | 11  | ARG  |
| 13  | AM    | 47  | ASP  |
| 13  | AM    | 64  | TRP  |
| 13  | AM    | 65  | LYS  |
| 13  | AM    | 91  | ARG  |
| 13  | AM    | 101 | GLN  |
| 13  | AM    | 108 | ARG  |
| 13  | AM    | 115 | LYS  |
| 14  | AN    | 14  | PRO  |
| 14  | AN    | 16  | PHE  |
| 14  | AN    | 23  | ARG  |
| 14  | AN    | 31  | ARG  |
| 14  | AN    | 33  | VAL  |
| 14  | AN    | 58  | LYS  |
| 15  | AO    | 25  | THR  |
| 15  | AO    | 31  | LEU  |
| 15  | AO    | 39  | LEU  |
| 15  | AO    | 56  | LEU  |
| 15  | AO    | 68  | ARG  |
| 15  | AO    | 74  | ASP  |
| 15  | AO    | 81  | LEU  |
| 15  | AO    | 82  | ILE  |
| 16  | AP    | 1   | MET  |
| 16  | AP    | 27  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | AP    | 55  | ARG  |
| 16  | AP    | 62  | VAL  |
| 17  | AQ    | 38  | ARG  |
| 17  | AQ    | 52  | LYS  |
| 18  | AR    | 31  | LEU  |
| 18  | AR    | 36  | ASN  |
| 18  | AR    | 47  | THR  |
| 18  | AR    | 50  | ILE  |
| 18  | AR    | 76  | LEU  |
| 18  | AR    | 86  | VAL  |
| 19  | AS    | 7   | LYS  |
| 19  | AS    | 12  | ASP  |
| 19  | AS    | 15  | LEU  |
| 19  | AS    | 21  | GLU  |
| 19  | AS    | 37  | ARG  |
| 19  | AS    | 62  | ILE  |
| 20  | AT    | 9   | ASN  |
| 20  | AT    | 18  | GLN  |
| 20  | AT    | 24  | LEU  |
| 20  | AT    | 26  | ASN  |
| 20  | AT    | 27  | LYS  |
| 20  | AT    | 41  | ILE  |
| 20  | AT    | 75  | ASN  |
| 20  | AT    | 82  | SER  |
| 21  | AU    | 15  | ARG  |
| 24  | AY    | 31  | ARG  |
| 24  | AY    | 40  | HIS  |
| 24  | AY    | 45  | VAL  |
| 24  | AY    | 52  | MET  |
| 24  | AY    | 54  | PHE  |
| 24  | AY    | 59  | ARG  |
| 24  | AY    | 60  | GLU  |
| 24  | AY    | 84  | THR  |
| 24  | AY    | 91  | THR  |
| 24  | AY    | 92  | ILE  |
| 24  | AY    | 98  | MET  |
| 24  | AY    | 101 | LEU  |
| 24  | AY    | 120 | THR  |
| 24  | AY    | 121 | VAL  |
| 24  | AY    | 128 | TYR  |
| 24  | AY    | 157 | LEU  |
| 24  | AY    | 191 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | AY    | 192 | LEU  |
| 24  | AY    | 224 | ASP  |
| 24  | AY    | 225 | GLU  |
| 24  | AY    | 232 | LEU  |
| 24  | AY    | 236 | GLU  |
| 24  | AY    | 252 | ASP  |
| 24  | AY    | 255 | ILE  |
| 24  | AY    | 260 | LEU  |
| 24  | AY    | 264 | LEU  |
| 24  | AY    | 277 | VAL  |
| 24  | AY    | 285 | ASP  |
| 24  | AY    | 289 | ILE  |
| 24  | AY    | 312 | LEU  |
| 24  | AY    | 343 | ASN  |
| 24  | AY    | 348 | ARG  |
| 24  | AY    | 356 | LEU  |
| 24  | AY    | 357 | ARG  |
| 24  | AY    | 369 | LEU  |
| 24  | AY    | 381 | LYS  |
| 24  | AY    | 417 | THR  |
| 24  | AY    | 420 | ASP  |
| 24  | AY    | 421 | GLN  |
| 24  | AY    | 426 | GLN  |
| 24  | AY    | 431 | LEU  |
| 24  | AY    | 437 | THR  |
| 24  | AY    | 458 | HIS  |
| 24  | AY    | 466 | LEU  |
| 24  | AY    | 478 | LYS  |
| 24  | AY    | 481 | VAL  |
| 24  | AY    | 487 | ILE  |
| 24  | AY    | 500 | GLN  |
| 24  | AY    | 504 | ARG  |
| 24  | AY    | 509 | HIS  |
| 24  | AY    | 512 | ILE  |
| 24  | AY    | 568 | TYR  |
| 24  | AY    | 572 | TYR  |
| 24  | AY    | 576 | ASP  |
| 24  | AY    | 580 | MET  |
| 24  | AY    | 607 | ARG  |
| 24  | AY    | 616 | TYR  |
| 24  | AY    | 623 | ASP  |
| 24  | AY    | 628 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | AY    | 635 | GLU  |
| 24  | AY    | 647 | VAL  |
| 24  | AY    | 649 | LEU  |
| 24  | AY    | 671 | MET  |
| 25  | B0    | 5   | LYS  |
| 25  | B0    | 11  | ARG  |
| 25  | B0    | 14  | ARG  |
| 25  | B0    | 20  | ARG  |
| 25  | B0    | 27  | GLU  |
| 25  | B0    | 30  | VAL  |
| 25  | B0    | 39  | ARG  |
| 25  | B0    | 40  | GLN  |
| 25  | B0    | 43  | THR  |
| 25  | B0    | 44  | ARG  |
| 25  | B0    | 53  | MET  |
| 25  | B0    | 55  | ARG  |
| 25  | B0    | 56  | ASP  |
| 25  | B0    | 57  | PHE  |
| 25  | B0    | 62  | LEU  |
| 25  | B0    | 69  | PHE  |
| 25  | B0    | 70  | GLN  |
| 25  | B0    | 74  | ARG  |
| 25  | B0    | 75  | LEU  |
| 25  | B0    | 80  | HIS  |
| 25  | B0    | 84  | LEU  |
| 26  | B1    | 5   | CYS  |
| 26  | B1    | 8   | SER  |
| 26  | B1    | 11  | ARG  |
| 26  | B1    | 25  | LYS  |
| 26  | B1    | 27  | GLU  |
| 26  | B1    | 30  | VAL  |
| 26  | B1    | 33  | LYS  |
| 26  | B1    | 37  | ILE  |
| 26  | B1    | 39  | LYS  |
| 26  | B1    | 40  | ARG  |
| 26  | B1    | 45  | ASN  |
| 26  | B1    | 50  | ARG  |
| 26  | B1    | 53  | VAL  |
| 26  | B1    | 73  | LEU  |
| 26  | B1    | 78  | LYS  |
| 26  | B1    | 80  | LEU  |
| 26  | B1    | 82  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | B1    | 83  | GLU  |
| 27  | B2    | 2   | LYS  |
| 27  | B2    | 4   | SER  |
| 27  | B2    | 7   | ARG  |
| 27  | B2    | 8   | LYS  |
| 27  | B2    | 9   | GLN  |
| 27  | B2    | 20  | GLU  |
| 27  | B2    | 24  | LEU  |
| 27  | B2    | 26  | ARG  |
| 27  | B2    | 27  | GLU  |
| 27  | B2    | 32  | LEU  |
| 27  | B2    | 37  | PHE  |
| 27  | B2    | 40  | SER  |
| 27  | B2    | 41  | ILE  |
| 27  | B2    | 43  | GLN  |
| 27  | B2    | 44  | LEU  |
| 27  | B2    | 45  | SER  |
| 27  | B2    | 47  | ASN  |
| 27  | B2    | 48  | HIS  |
| 27  | B2    | 49  | LYS  |
| 27  | B2    | 51  | ARG  |
| 27  | B2    | 53  | LEU  |
| 27  | B2    | 65  | ASN  |
| 27  | B2    | 68  | ARG  |
| 27  | B2    | 70  | GLN  |
| 28  | B3    | 8   | LEU  |
| 28  | B3    | 10  | LYS  |
| 28  | B3    | 29  | ARG  |
| 28  | B3    | 30  | ARG  |
| 28  | B3    | 33  | GLN  |
| 28  | B3    | 55  | ARG  |
| 28  | B3    | 57  | GLU  |
| 29  | B4    | 1   | MET  |
| 29  | B4    | 24  | THR  |
| 29  | B4    | 25  | TYR  |
| 29  | B4    | 27  | THR  |
| 29  | B4    | 31  | ILE  |
| 29  | B4    | 38  | LYS  |
| 29  | B4    | 39  | CYS  |
| 29  | B4    | 42  | PHE  |
| 29  | B4    | 49  | PHE  |
| 29  | B4    | 52  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | B4    | 53  | GLU  |
| 29  | B4    | 58  | ARG  |
| 29  | B4    | 59  | PHE  |
| 29  | B4    | 61  | ARG  |
| 29  | B4    | 62  | ARG  |
| 30  | B5    | 3   | LYS  |
| 30  | B5    | 4   | HIS  |
| 30  | B5    | 26  | THR  |
| 30  | B5    | 29  | THR  |
| 30  | B5    | 44  | THR  |
| 30  | B5    | 48  | GLU  |
| 30  | B5    | 51  | TYR  |
| 30  | B5    | 52  | TYR  |
| 30  | B5    | 55  | ARG  |
| 31  | B6    | 7   | ILE  |
| 31  | B6    | 8   | LYS  |
| 31  | B6    | 9   | LEU  |
| 31  | B6    | 10  | LEU  |
| 31  | B6    | 11  | LEU  |
| 31  | B6    | 18  | ARG  |
| 31  | B6    | 29  | ASN  |
| 31  | B6    | 31  | PRO  |
| 31  | B6    | 35  | GLU  |
| 31  | B6    | 42  | TRP  |
| 31  | B6    | 45  | LYS  |
| 31  | B6    | 53  | LYS  |
| 32  | B7    | 8   | ASN  |
| 32  | B7    | 43  | THR  |
| 33  | B8    | 13  | ARG  |
| 33  | B8    | 19  | SER  |
| 33  | B8    | 30  | ARG  |
| 33  | B8    | 31  | HIS  |
| 33  | B8    | 32  | LEU  |
| 33  | B8    | 34  | TRP  |
| 33  | B8    | 41  | ILE  |
| 33  | B8    | 44  | LYS  |
| 33  | B8    | 47  | LYS  |
| 33  | B8    | 49  | VAL  |
| 33  | B8    | 61  | LEU  |
| 34  | B9    | 2   | LYS  |
| 34  | B9    | 11  | CYS  |
| 34  | B9    | 29  | ASN  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 37         | BC           | 28         | ARG         |
| 37         | BC           | 32         | GLU         |
| 37         | BC           | 48         | LEU         |
| 37         | BC           | 50         | ILE         |
| 37         | BC           | 53         | ARG         |
| 37         | BC           | 54         | ARG         |
| 37         | BC           | 98         | GLU         |
| 37         | BC           | 99         | GLU         |
| 37         | BC           | 103        | LYS         |
| 37         | BC           | 106        | ASP         |
| 37         | BC           | 108        | TRP         |
| 37         | BC           | 119        | ASP         |
| 37         | BC           | 121        | MET         |
| 37         | BC           | 127        | LYS         |
| 37         | BC           | 130        | ARG         |
| 37         | BC           | 138        | LEU         |
| 37         | BC           | 148        | PHE         |
| 37         | BC           | 158        | LYS         |
| 37         | BC           | 203        | GLU         |
| 38         | BD           | 3          | VAL         |
| 38         | BD           | 4          | LYS         |
| 38         | BD           | 18         | VAL         |
| 38         | BD           | 24         | ILE         |
| 38         | BD           | 25         | THR         |
| 38         | BD           | 26         | LYS         |
| 38         | BD           | 35         | LYS         |
| 38         | BD           | 46         | GLN         |
| 38         | BD           | 64         | ILE         |
| 38         | BD           | 65         | ILE         |
| 38         | BD           | 89         | SER         |
| 38         | BD           | 95         | LEU         |
| 38         | BD           | 98         | VAL         |
| 38         | BD           | 105        | ILE         |
| 38         | BD           | 106        | ILE         |
| 38         | BD           | 122        | ASP         |
| 38         | BD           | 131        | LEU         |
| 38         | BD           | 141        | VAL         |
| 38         | BD           | 155        | LEU         |
| 38         | BD           | 166        | GLN         |
| 38         | BD           | 173        | VAL         |
| 38         | BD           | 176        | ARG         |
| 38         | BD           | 192        | THR         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BD    | 211 | ARG  |
| 38  | BD    | 212 | SER  |
| 38  | BD    | 218 | ARG  |
| 38  | BD    | 221 | VAL  |
| 38  | BD    | 229 | VAL  |
| 38  | BD    | 242 | ARG  |
| 38  | BD    | 257 | LEU  |
| 38  | BD    | 259 | THR  |
| 38  | BD    | 270 | ILE  |
| 39  | BE    | 9   | VAL  |
| 39  | BE    | 47  | VAL  |
| 39  | BE    | 49  | LEU  |
| 39  | BE    | 52  | LEU  |
| 39  | BE    | 54  | GLN  |
| 39  | BE    | 55  | ASN  |
| 39  | BE    | 56  | PRO  |
| 39  | BE    | 57  | LYS  |
| 39  | BE    | 63  | LEU  |
| 39  | BE    | 67  | PHE  |
| 39  | BE    | 69  | LYS  |
| 39  | BE    | 76  | ARG  |
| 39  | BE    | 79  | ARG  |
| 39  | BE    | 82  | ARG  |
| 39  | BE    | 87  | GLU  |
| 39  | BE    | 93  | VAL  |
| 39  | BE    | 94  | GLU  |
| 39  | BE    | 111 | ARG  |
| 39  | BE    | 116 | VAL  |
| 39  | BE    | 121 | ASN  |
| 39  | BE    | 134 | ILE  |
| 39  | BE    | 144 | ARG  |
| 39  | BE    | 146 | THR  |
| 39  | BE    | 154 | LYS  |
| 39  | BE    | 167 | VAL  |
| 39  | BE    | 169 | ASN  |
| 39  | BE    | 175 | VAL  |
| 39  | BE    | 178 | GLU  |
| 39  | BE    | 185 | LYS  |
| 39  | BE    | 197 | ILE  |
| 39  | BE    | 202 | LYS  |
| 39  | BE    | 203 | LYS  |
| 40  | BF    | 17  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BF    | 19  | GLU  |
| 40  | BF    | 20  | LEU  |
| 40  | BF    | 28  | ILE  |
| 40  | BF    | 33  | LEU  |
| 40  | BF    | 35  | GLU  |
| 40  | BF    | 50  | SER  |
| 40  | BF    | 65  | TRP  |
| 40  | BF    | 68  | LYS  |
| 40  | BF    | 82  | ILE  |
| 40  | BF    | 110 | LEU  |
| 40  | BF    | 122 | LYS  |
| 40  | BF    | 125 | LEU  |
| 40  | BF    | 157 | VAL  |
| 40  | BF    | 158 | THR  |
| 40  | BF    | 160 | ASN  |
| 40  | BF    | 164 | ARG  |
| 40  | BF    | 169 | ASN  |
| 40  | BF    | 179 | GLU  |
| 41  | BG    | 9   | ARG  |
| 41  | BG    | 13  | GLU  |
| 41  | BG    | 21  | ARG  |
| 41  | BG    | 22  | ARG  |
| 41  | BG    | 26  | GLN  |
| 41  | BG    | 27  | ASN  |
| 41  | BG    | 33  | ARG  |
| 41  | BG    | 45  | GLU  |
| 41  | BG    | 48  | GLU  |
| 41  | BG    | 60  | LEU  |
| 41  | BG    | 66  | GLN  |
| 41  | BG    | 79  | ASN  |
| 41  | BG    | 82  | LEU  |
| 41  | BG    | 83  | ARG  |
| 41  | BG    | 91  | ARG  |
| 41  | BG    | 95  | ARG  |
| 41  | BG    | 106 | LEU  |
| 41  | BG    | 107 | LEU  |
| 41  | BG    | 108 | ASN  |
| 41  | BG    | 113 | ARG  |
| 41  | BG    | 118 | ARG  |
| 41  | BG    | 121 | ASN  |
| 41  | BG    | 133 | LEU  |
| 41  | BG    | 135 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BG    | 136 | ARG  |
| 41  | BG    | 139 | LEU  |
| 41  | BG    | 146 | TYR  |
| 41  | BG    | 176 | LEU  |
| 41  | BG    | 180 | PHE  |
| 41  | BG    | 182 | LYS  |
| 42  | BH    | 1   | MET  |
| 42  | BH    | 3   | ARG  |
| 42  | BH    | 6   | ARG  |
| 42  | BH    | 9   | ILE  |
| 42  | BH    | 47  | GLU  |
| 42  | BH    | 69  | ARG  |
| 42  | BH    | 83  | TYR  |
| 42  | BH    | 89  | ILE  |
| 42  | BH    | 104 | GLU  |
| 42  | BH    | 105 | LEU  |
| 42  | BH    | 111 | HIS  |
| 42  | BH    | 158 | HIS  |
| 42  | BH    | 159 | GLU  |
| 42  | BH    | 168 | PRO  |
| 42  | BH    | 170 | ARG  |
| 46  | BN    | 1   | MET  |
| 46  | BN    | 2   | LYS  |
| 46  | BN    | 25  | ARG  |
| 46  | BN    | 33  | LEU  |
| 46  | BN    | 34  | LEU  |
| 46  | BN    | 35  | ARG  |
| 46  | BN    | 45  | ASN  |
| 46  | BN    | 48  | MET  |
| 46  | BN    | 50  | ASP  |
| 46  | BN    | 68  | GLU  |
| 46  | BN    | 119 | ARG  |
| 46  | BN    | 129 | PRO  |
| 46  | BN    | 131 | GLN  |
| 46  | BN    | 136 | GLU  |
| 47  | BO    | 13  | ASN  |
| 47  | BO    | 22  | ILE  |
| 47  | BO    | 23  | ARG  |
| 47  | BO    | 24  | VAL  |
| 47  | BO    | 47  | ILE  |
| 47  | BO    | 49  | ARG  |
| 47  | BO    | 52  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | BP    | 6   | LEU  |
| 48  | BP    | 9   | ASN  |
| 48  | BP    | 16  | ARG  |
| 48  | BP    | 18  | ARG  |
| 48  | BP    | 33  | ARG  |
| 48  | BP    | 35  | HIS  |
| 48  | BP    | 39  | LYS  |
| 48  | BP    | 41  | ARG  |
| 48  | BP    | 47  | ASP  |
| 48  | BP    | 49  | ARG  |
| 48  | BP    | 51  | PHE  |
| 48  | BP    | 52  | GLU  |
| 48  | BP    | 55  | ARG  |
| 48  | BP    | 57  | THR  |
| 48  | BP    | 59  | LEU  |
| 48  | BP    | 61  | ARG  |
| 48  | BP    | 62  | LEU  |
| 48  | BP    | 68  | GLN  |
| 48  | BP    | 70  | GLN  |
| 48  | BP    | 85  | LEU  |
| 48  | BP    | 91  | PHE  |
| 48  | BP    | 105 | LEU  |
| 48  | BP    | 108 | LYS  |
| 48  | BP    | 110 | TYR  |
| 48  | BP    | 111 | ARG  |
| 48  | BP    | 115 | LEU  |
| 48  | BP    | 119 | GLU  |
| 48  | BP    | 135 | LEU  |
| 49  | BQ    | 1   | MET  |
| 49  | BQ    | 14  | ARG  |
| 49  | BQ    | 16  | ARG  |
| 49  | BQ    | 45  | GLN  |
| 49  | BQ    | 51  | ARG  |
| 49  | BQ    | 54  | MET  |
| 49  | BQ    | 56  | ARG  |
| 49  | BQ    | 59  | ARG  |
| 49  | BQ    | 65  | PHE  |
| 49  | BQ    | 74  | TYR  |
| 49  | BQ    | 75  | THR  |
| 49  | BQ    | 79  | LEU  |
| 49  | BQ    | 110 | THR  |
| 49  | BQ    | 133 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | BQ    | 141 | GLN  |
| 50  | BR    | 2   | ARG  |
| 50  | BR    | 8   | ARG  |
| 50  | BR    | 10  | LEU  |
| 50  | BR    | 11  | ASN  |
| 50  | BR    | 16  | HIS  |
| 50  | BR    | 18  | LEU  |
| 50  | BR    | 28  | LEU  |
| 50  | BR    | 29  | LEU  |
| 50  | BR    | 34  | ILE  |
| 50  | BR    | 71  | GLN  |
| 50  | BR    | 83  | ILE  |
| 50  | BR    | 89  | ASP  |
| 50  | BR    | 99  | LYS  |
| 50  | BR    | 100 | LEU  |
| 50  | BR    | 113 | LEU  |
| 50  | BR    | 116 | LEU  |
| 50  | BR    | 117 | VAL  |
| 50  | BR    | 118 | GLU  |
| 51  | BS    | 11  | LYS  |
| 51  | BS    | 12  | PHE  |
| 51  | BS    | 15  | ARG  |
| 51  | BS    | 17  | ARG  |
| 51  | BS    | 20  | ARG  |
| 51  | BS    | 29  | PHE  |
| 51  | BS    | 36  | TYR  |
| 51  | BS    | 40  | ILE  |
| 51  | BS    | 54  | LEU  |
| 51  | BS    | 56  | LEU  |
| 51  | BS    | 59  | LYS  |
| 51  | BS    | 64  | GLU  |
| 51  | BS    | 92  | TYR  |
| 51  | BS    | 97  | ARG  |
| 51  | BS    | 106 | ARG  |
| 52  | BT    | 2   | ASN  |
| 52  | BT    | 7   | ILE  |
| 52  | BT    | 16  | ARG  |
| 52  | BT    | 23  | ARG  |
| 52  | BT    | 28  | VAL  |
| 52  | BT    | 29  | ARG  |
| 52  | BT    | 30  | VAL  |
| 52  | BT    | 33  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | BT    | 38  | ASN  |
| 52  | BT    | 41  | ARG  |
| 52  | BT    | 49  | VAL  |
| 52  | BT    | 51  | ARG  |
| 52  | BT    | 58  | ASN  |
| 52  | BT    | 59  | THR  |
| 52  | BT    | 78  | LEU  |
| 52  | BT    | 79  | HIS  |
| 52  | BT    | 80  | SER  |
| 52  | BT    | 83  | ILE  |
| 52  | BT    | 95  | ARG  |
| 52  | BT    | 96  | ARG  |
| 52  | BT    | 99  | LEU  |
| 52  | BT    | 111 | ARG  |
| 52  | BT    | 118 | ARG  |
| 52  | BT    | 124 | ASP  |
| 52  | BT    | 132 | LYS  |
| 52  | BT    | 133 | GLU  |
| 53  | BU    | 8   | VAL  |
| 53  | BU    | 14  | HIS  |
| 53  | BU    | 18  | LEU  |
| 53  | BU    | 56  | ASP  |
| 53  | BU    | 59  | ARG  |
| 53  | BU    | 60  | LEU  |
| 53  | BU    | 66  | ASN  |
| 53  | BU    | 74  | LEU  |
| 53  | BU    | 84  | LYS  |
| 53  | BU    | 92  | ARG  |
| 53  | BU    | 101 | ARG  |
| 53  | BU    | 108 | GLU  |
| 54  | BV    | 1   | MET  |
| 54  | BV    | 2   | PHE  |
| 54  | BV    | 7   | THR  |
| 54  | BV    | 10  | LYS  |
| 54  | BV    | 12  | TYR  |
| 54  | BV    | 16  | PRO  |
| 54  | BV    | 18  | LEU  |
| 54  | BV    | 19  | LYS  |
| 54  | BV    | 21  | ARG  |
| 54  | BV    | 35  | LEU  |
| 54  | BV    | 39  | LEU  |
| 54  | BV    | 40  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BV    | 45  | THR  |
| 54  | BV    | 50  | PRO  |
| 54  | BV    | 71  | LEU  |
| 54  | BV    | 89  | GLN  |
| 54  | BV    | 99  | ILE  |
| 55  | BW    | 11  | ARG  |
| 55  | BW    | 21  | VAL  |
| 55  | BW    | 23  | LEU  |
| 55  | BW    | 36  | LEU  |
| 55  | BW    | 50  | VAL  |
| 55  | BW    | 76  | VAL  |
| 55  | BW    | 78  | GLU  |
| 55  | BW    | 90  | ARG  |
| 55  | BW    | 95  | ILE  |
| 55  | BW    | 96  | ILE  |
| 55  | BW    | 104 | THR  |
| 55  | BW    | 106 | ILE  |
| 56  | BX    | 27  | THR  |
| 56  | BX    | 57  | LEU  |
| 56  | BX    | 68  | ARG  |
| 56  | BX    | 70  | LEU  |
| 56  | BX    | 80  | ILE  |
| 56  | BX    | 90  | GLU  |
| 57  | BY    | 2   | ARG  |
| 57  | BY    | 6   | HIS  |
| 57  | BY    | 23  | ARG  |
| 57  | BY    | 28  | LYS  |
| 57  | BY    | 29  | GLU  |
| 57  | BY    | 32  | PRO  |
| 57  | BY    | 38  | ILE  |
| 57  | BY    | 53  | PRO  |
| 57  | BY    | 55  | TYR  |
| 57  | BY    | 56  | PRO  |
| 57  | BY    | 77  | PRO  |
| 57  | BY    | 83  | THR  |
| 57  | BY    | 85  | VAL  |
| 57  | BY    | 88  | LYS  |
| 57  | BY    | 89  | PHE  |
| 57  | BY    | 90  | LEU  |
| 57  | BY    | 95  | LYS  |
| 57  | BY    | 97  | ARG  |
| 57  | BY    | 99  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | BZ    | 6   | LYS  |
| 58  | BZ    | 20  | ARG  |
| 58  | BZ    | 32  | HIS  |
| 58  | BZ    | 41  | LEU  |
| 58  | BZ    | 44  | PHE  |
| 58  | BZ    | 48  | PHE  |
| 58  | BZ    | 67  | LEU  |
| 58  | BZ    | 70  | LEU  |
| 58  | BZ    | 72  | ARG  |
| 58  | BZ    | 81  | ARG  |
| 58  | BZ    | 97  | GLU  |
| 58  | BZ    | 103 | ARG  |
| 58  | BZ    | 112 | ARG  |
| 58  | BZ    | 121 | HIS  |
| 58  | BZ    | 122 | ARG  |
| 58  | BZ    | 140 | ASP  |
| 58  | BZ    | 148 | ASP  |
| 58  | BZ    | 155 | LEU  |
| 58  | BZ    | 163 | LEU  |
| 58  | BZ    | 168 | GLU  |
| 58  | BZ    | 182 | LYS  |
| 58  | BZ    | 183 | LEU  |
| 58  | BZ    | 185 | GLU  |
| 58  | BZ    | 186 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 37  | ASN  |
| 2   | AB    | 45  | GLN  |
| 2   | AB    | 78  | GLN  |
| 2   | AB    | 146 | GLN  |
| 2   | AB    | 204 | ASN  |
| 2   | AB    | 212 | GLN  |
| 3   | AC    | 63  | ASN  |
| 3   | AC    | 110 | ASN  |
| 3   | AC    | 123 | GLN  |
| 3   | AC    | 170 | GLN  |
| 3   | AC    | 176 | HIS  |
| 3   | AC    | 181 | ASN  |
| 4   | AD    | 62  | GLN  |
| 4   | AD    | 77  | ASN  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 4          | AD           | 129        | ASN         |
| 5          | AE           | 20         | GLN         |
| 5          | AE           | 38         | GLN         |
| 5          | AE           | 73         | ASN         |
| 6          | AF           | 16         | GLN         |
| 6          | AF           | 18         | GLN         |
| 6          | AF           | 27         | GLN         |
| 6          | AF           | 32         | ASN         |
| 6          | AF           | 57         | GLN         |
| 6          | AF           | 73         | ASN         |
| 6          | AF           | 84         | ASN         |
| 6          | AF           | 94         | GLN         |
| 6          | AF           | 100        | ASN         |
| 7          | AG           | 64         | GLN         |
| 7          | AG           | 68         | ASN         |
| 7          | AG           | 84         | ASN         |
| 7          | AG           | 122        | HIS         |
| 7          | AG           | 153        | HIS         |
| 9          | AI           | 23         | ASN         |
| 9          | AI           | 34         | ASN         |
| 9          | AI           | 124        | GLN         |
| 10         | AJ           | 56         | HIS         |
| 10         | AJ           | 78         | ASN         |
| 12         | AL           | 8          | ASN         |
| 12         | AL           | 9          | GLN         |
| 12         | AL           | 49         | ASN         |
| 12         | AL           | 75         | HIS         |
| 12         | AL           | 78         | GLN         |
| 13         | AM           | 12         | ASN         |
| 13         | AM           | 40         | ASN         |
| 13         | AM           | 62         | ASN         |
| 13         | AM           | 77         | ASN         |
| 13         | AM           | 101        | GLN         |
| 14         | AN           | 49         | HIS         |
| 15         | AO           | 37         | ASN         |
| 15         | AO           | 46         | HIS         |
| 15         | AO           | 71         | GLN         |
| 16         | AP           | 16         | HIS         |
| 16         | AP           | 76         | GLN         |
| 17         | AQ           | 16         | GLN         |
| 18         | AR           | 36         | ASN         |
| 19         | AS           | 47         | HIS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 19         | AS           | 53         | ASN         |
| 19         | AS           | 65         | ASN         |
| 20         | AT           | 18         | GLN         |
| 20         | AT           | 26         | ASN         |
| 20         | AT           | 73         | HIS         |
| 20         | AT           | 75         | ASN         |
| 24         | AY           | 14         | ASN         |
| 24         | AY           | 137        | ASN         |
| 24         | AY           | 165        | GLN         |
| 24         | AY           | 208        | GLN         |
| 24         | AY           | 270        | GLN         |
| 24         | AY           | 343        | ASN         |
| 24         | AY           | 421        | GLN         |
| 24         | AY           | 458        | HIS         |
| 24         | AY           | 543        | GLN         |
| 24         | AY           | 625        | ASN         |
| 24         | AY           | 641        | GLN         |
| 24         | AY           | 664        | GLN         |
| 24         | AY           | 684        | GLN         |
| 25         | B0           | 17         | GLN         |
| 25         | B0           | 29         | GLN         |
| 25         | B0           | 50         | ASN         |
| 25         | B0           | 70         | GLN         |
| 26         | B1           | 19         | GLN         |
| 26         | B1           | 45         | ASN         |
| 27         | B2           | 46         | GLN         |
| 27         | B2           | 47         | ASN         |
| 27         | B2           | 70         | GLN         |
| 28         | B3           | 19         | GLN         |
| 28         | B3           | 46         | ASN         |
| 28         | B3           | 52         | HIS         |
| 30         | B5           | 23         | HIS         |
| 31         | B6           | 32         | ASN         |
| 32         | B7           | 8          | ASN         |
| 34         | B9           | 34         | GLN         |
| 37         | BC           | 67         | HIS         |
| 37         | BC           | 72         | GLN         |
| 37         | BC           | 149        | ASN         |
| 37         | BC           | 189        | ASN         |
| 37         | BC           | 200        | HIS         |
| 38         | BD           | 96         | HIS         |
| 38         | BD           | 115        | GLN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BD    | 116 | GLN  |
| 38  | BD    | 126 | GLN  |
| 38  | BD    | 166 | GLN  |
| 38  | BD    | 186 | HIS  |
| 38  | BD    | 198 | ASN  |
| 38  | BD    | 201 | HIS  |
| 39  | BE    | 48  | GLN  |
| 39  | BE    | 54  | GLN  |
| 39  | BE    | 55  | ASN  |
| 39  | BE    | 129 | HIS  |
| 39  | BE    | 143 | ASN  |
| 39  | BE    | 169 | ASN  |
| 39  | BE    | 192 | ASN  |
| 40  | BF    | 69  | HIS  |
| 40  | BF    | 133 | ASN  |
| 40  | BF    | 160 | ASN  |
| 40  | BF    | 169 | ASN  |
| 40  | BF    | 204 | ASN  |
| 41  | BG    | 27  | ASN  |
| 41  | BG    | 66  | GLN  |
| 41  | BG    | 108 | ASN  |
| 42  | BH    | 65  | HIS  |
| 42  | BH    | 74  | ASN  |
| 42  | BH    | 139 | GLN  |
| 42  | BH    | 147 | ASN  |
| 42  | BH    | 158 | HIS  |
| 46  | BN    | 45  | ASN  |
| 46  | BN    | 56  | ASN  |
| 46  | BN    | 128 | HIS  |
| 47  | BO    | 13  | ASN  |
| 47  | BO    | 82  | ASN  |
| 48  | BP    | 27  | HIS  |
| 48  | BP    | 38  | GLN  |
| 48  | BP    | 68  | GLN  |
| 48  | BP    | 81  | GLN  |
| 48  | BP    | 84  | ASN  |
| 48  | BP    | 128 | HIS  |
| 49  | BQ    | 13  | GLN  |
| 49  | BQ    | 45  | GLN  |
| 49  | BQ    | 57  | HIS  |
| 49  | BQ    | 141 | GLN  |
| 50  | BR    | 3   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | BR    | 11  | ASN  |
| 50  | BR    | 13  | HIS  |
| 50  | BR    | 23  | ASN  |
| 50  | BR    | 53  | HIS  |
| 50  | BR    | 61  | HIS  |
| 50  | BR    | 71  | GLN  |
| 51  | BS    | 34  | HIS  |
| 52  | BT    | 38  | ASN  |
| 52  | BT    | 43  | GLN  |
| 52  | BT    | 79  | HIS  |
| 52  | BT    | 90  | GLN  |
| 53  | BU    | 14  | HIS  |
| 53  | BU    | 49  | HIS  |
| 53  | BU    | 66  | ASN  |
| 53  | BU    | 81  | HIS  |
| 53  | BU    | 94  | ASN  |
| 53  | BU    | 117 | GLN  |
| 54  | BV    | 11  | GLN  |
| 55  | BW    | 34  | ASN  |
| 55  | BW    | 57  | ASN  |
| 55  | BW    | 102 | HIS  |
| 56  | BX    | 31  | HIS  |
| 56  | BX    | 41  | ASN  |
| 56  | BX    | 87  | GLN  |
| 58  | BZ    | 34  | ASN  |
| 58  | BZ    | 54  | HIS  |
| 58  | BZ    | 65  | GLN  |
| 58  | BZ    | 132 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1505/1519 (99%) | 320 (21%)         | 51 (3%)         |
| 22  | AV    | 75/76 (98%)     | 24 (32%)          | 2 (2%)          |
| 23  | AX    | 8/9 (88%)       | 3 (37%)           | 0               |
| 35  | BA    | 2897/2915 (99%) | 665 (22%)         | 60 (2%)         |
| 36  | BB    | 118/122 (96%)   | 26 (22%)          | 2 (1%)          |
| All | All   | 4603/4641 (99%) | 1038 (22%)        | 115 (2%)        |

All (1038) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | AA    | 9      | G    |
| 1   | AA    | 31     | G    |
| 1   | AA    | 32     | A    |
| 1   | AA    | 38     | G    |
| 1   | AA    | 39     | G    |
| 1   | AA    | 40     | C    |
| 1   | AA    | 48     | C    |
| 1   | AA    | 51     | A    |
| 1   | AA    | 57     | G    |
| 1   | AA    | 60     | A    |
| 1   | AA    | 61     | G    |
| 1   | AA    | 64     | G    |
| 1   | AA    | 65     | U    |
| 1   | AA    | 76     | C    |
| 1   | AA    | 77     | G    |
| 1   | AA    | 78     | G    |
| 1   | AA    | 79     | G    |
| 1   | AA    | 80     | G    |
| 1   | AA    | 81     | U    |
| 1   | AA    | 82     | U    |
| 1   | AA    | 83     | U    |
| 1   | AA    | 84     | U    |
| 1   | AA    | 88     | A    |
| 1   | AA    | 89     | C    |
| 1   | AA    | 90     | U    |
| 1   | AA    | 91     | C    |
| 1   | AA    | 92     | C    |
| 1   | AA    | 101    | A    |
| 1   | AA    | 107    | G    |
| 1   | AA    | 108    | G    |
| 1   | AA    | 113    | G    |
| 1   | AA    | 116    | A    |
| 1   | AA    | 120    | A    |
| 1   | AA    | 121    | C    |
| 1   | AA    | 131    | C    |
| 1   | AA    | 144    | G    |
| 1   | AA    | 189(H) | G    |
| 1   | AA    | 189(I) | G    |
| 1   | AA    | 195    | A    |
| 1   | AA    | 197    | A    |
| 1   | AA    | 198    | G    |
| 1   | AA    | 199    | G    |
| 1   | AA    | 203    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 204 | U    |
| 1   | AA    | 244 | U    |
| 1   | AA    | 247 | G    |
| 1   | AA    | 251 | G    |
| 1   | AA    | 265 | G    |
| 1   | AA    | 266 | G    |
| 1   | AA    | 267 | C    |
| 1   | AA    | 268 | C    |
| 1   | AA    | 275 | G    |
| 1   | AA    | 289 | G    |
| 1   | AA    | 312 | C    |
| 1   | AA    | 321 | A    |
| 1   | AA    | 324 | G    |
| 1   | AA    | 328 | C    |
| 1   | AA    | 332 | G    |
| 1   | AA    | 345 | C    |
| 1   | AA    | 346 | G    |
| 1   | AA    | 347 | G    |
| 1   | AA    | 348 | G    |
| 1   | AA    | 349 | A    |
| 1   | AA    | 352 | C    |
| 1   | AA    | 353 | A    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 365 | U    |
| 1   | AA    | 366 | C    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 372 | C    |
| 1   | AA    | 384 | G    |
| 1   | AA    | 389 | A    |
| 1   | AA    | 397 | A    |
| 1   | AA    | 398 | C    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 413 | G    |
| 1   | AA    | 414 | A    |
| 1   | AA    | 421 | U    |
| 1   | AA    | 422 | C    |
| 1   | AA    | 423 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 442 | C    |
| 1   | AA    | 452 | A    |
| 1   | AA    | 453 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 454 | C    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | G    |
| 1   | AA    | 491 | G    |
| 1   | AA    | 496 | A    |
| 1   | AA    | 499 | A    |
| 1   | AA    | 505 | G    |
| 1   | AA    | 507 | C    |
| 1   | AA    | 508 | C    |
| 1   | AA    | 509 | A    |
| 1   | AA    | 510 | A    |
| 1   | AA    | 511 | C    |
| 1   | AA    | 518 | C    |
| 1   | AA    | 522 | C    |
| 1   | AA    | 527 | G    |
| 1   | AA    | 531 | U    |
| 1   | AA    | 532 | A    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 544 | G    |
| 1   | AA    | 546 | G    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 548 | G    |
| 1   | AA    | 557 | G    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 560 | U    |
| 1   | AA    | 561 | U    |
| 1   | AA    | 562 | C    |
| 1   | AA    | 563 | A    |
| 1   | AA    | 564 | C    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 576 | G    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 588 | G    |
| 1   | AA    | 589 | C    |
| 1   | AA    | 590 | C    |
| 1   | AA    | 593 | G    |
| 1   | AA    | 595 | G    |
| 1   | AA    | 632 | A    |
| 1   | AA    | 633 | G    |
| 1   | AA    | 653 | A    |
| 1   | AA    | 665 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 686 | U    |
| 1   | AA    | 687 | A    |
| 1   | AA    | 688 | G    |
| 1   | AA    | 700 | G    |
| 1   | AA    | 702 | A    |
| 1   | AA    | 703 | G    |
| 1   | AA    | 705 | U    |
| 1   | AA    | 722 | A    |
| 1   | AA    | 723 | U    |
| 1   | AA    | 731 | G    |
| 1   | AA    | 749 | C    |
| 1   | AA    | 755 | G    |
| 1   | AA    | 770 | C    |
| 1   | AA    | 771 | G    |
| 1   | AA    | 774 | G    |
| 1   | AA    | 777 | A    |
| 1   | AA    | 788 | U    |
| 1   | AA    | 792 | A    |
| 1   | AA    | 793 | U    |
| 1   | AA    | 794 | A    |
| 1   | AA    | 796 | C    |
| 1   | AA    | 816 | A    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 828 | A    |
| 1   | AA    | 839 | U    |
| 1   | AA    | 840 | C    |
| 1   | AA    | 841 | U    |
| 1   | AA    | 848 | C    |
| 1   | AA    | 859 | A    |
| 1   | AA    | 861 | G    |
| 1   | AA    | 863 | U    |
| 1   | AA    | 868 | C    |
| 1   | AA    | 872 | A    |
| 1   | AA    | 874 | G    |
| 1   | AA    | 902 | G    |
| 1   | AA    | 917 | G    |
| 1   | AA    | 922 | G    |
| 1   | AA    | 926 | G    |
| 1   | AA    | 927 | G    |
| 1   | AA    | 934 | C    |
| 1   | AA    | 935 | A    |
| 1   | AA    | 939 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 940     | C    |
| 1   | AA    | 941     | G    |
| 1   | AA    | 948     | C    |
| 1   | AA    | 950     | U    |
| 1   | AA    | 951     | G    |
| 1   | AA    | 952     | U    |
| 1   | AA    | 953     | G    |
| 1   | AA    | 957     | U    |
| 1   | AA    | 960     | U    |
| 1   | AA    | 961     | U    |
| 1   | AA    | 962     | C    |
| 1   | AA    | 963     | G    |
| 1   | AA    | 966     | G    |
| 1   | AA    | 968     | A    |
| 1   | AA    | 969     | A    |
| 1   | AA    | 974     | A    |
| 1   | AA    | 975     | A    |
| 1   | AA    | 976     | G    |
| 1   | AA    | 977     | A    |
| 1   | AA    | 980     | C    |
| 1   | AA    | 981     | U    |
| 1   | AA    | 982     | U    |
| 1   | AA    | 983     | A    |
| 1   | AA    | 992     | U    |
| 1   | AA    | 993     | G    |
| 1   | AA    | 996     | A    |
| 1   | AA    | 1001(A) | G    |
| 1   | AA    | 1004    | A    |
| 1   | AA    | 1025    | U    |
| 1   | AA    | 1028    | C    |
| 1   | AA    | 1029    | C    |
| 1   | AA    | 1030    | C    |
| 1   | AA    | 1030(C) | G    |
| 1   | AA    | 1031    | G    |
| 1   | AA    | 1048    | G    |
| 1   | AA    | 1050    | G    |
| 1   | AA    | 1054    | C    |
| 1   | AA    | 1066    | C    |
| 1   | AA    | 1072    | G    |
| 1   | AA    | 1074    | G    |
| 1   | AA    | 1076    | C    |
| 1   | AA    | 1078    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1081 | G    |
| 1   | AA    | 1094 | G    |
| 1   | AA    | 1095 | U    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1102 | A    |
| 1   | AA    | 1117 | G    |
| 1   | AA    | 1125 | U    |
| 1   | AA    | 1129 | C    |
| 1   | AA    | 1130 | A    |
| 1   | AA    | 1131 | G    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1138 | G    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1140 | C    |
| 1   | AA    | 1141 | C    |
| 1   | AA    | 1145 | C    |
| 1   | AA    | 1151 | A    |
| 1   | AA    | 1152 | A    |
| 1   | AA    | 1154 | G    |
| 1   | AA    | 1158 | C    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1176 | A    |
| 1   | AA    | 1182 | G    |
| 1   | AA    | 1183 | A    |
| 1   | AA    | 1184 | G    |
| 1   | AA    | 1185 | G    |
| 1   | AA    | 1187 | G    |
| 1   | AA    | 1190 | G    |
| 1   | AA    | 1195 | C    |
| 1   | AA    | 1196 | U    |
| 1   | AA    | 1197 | G    |
| 1   | AA    | 1200 | C    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1212 | U    |
| 1   | AA    | 1213 | A    |
| 1   | AA    | 1227 | A    |
| 1   | AA    | 1229 | A    |
| 1   | AA    | 1238 | A    |
| 1   | AA    | 1240 | U    |
| 1   | AA    | 1241 | G    |
| 1   | AA    | 1256 | A    |
| 1   | AA    | 1257 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1267 | C    |
| 1   | AA    | 1268 | A    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1281 | U    |
| 1   | AA    | 1283 | G    |
| 1   | AA    | 1284 | C    |
| 1   | AA    | 1285 | A    |
| 1   | AA    | 1286 | A    |
| 1   | AA    | 1287 | A    |
| 1   | AA    | 1299 | A    |
| 1   | AA    | 1300 | G    |
| 1   | AA    | 1302 | U    |
| 1   | AA    | 1305 | G    |
| 1   | AA    | 1317 | C    |
| 1   | AA    | 1320 | C    |
| 1   | AA    | 1322 | C    |
| 1   | AA    | 1323 | G    |
| 1   | AA    | 1331 | G    |
| 1   | AA    | 1335 | C    |
| 1   | AA    | 1338 | G    |
| 1   | AA    | 1346 | A    |
| 1   | AA    | 1347 | G    |
| 1   | AA    | 1353 | G    |
| 1   | AA    | 1364 | U    |
| 1   | AA    | 1369 | C    |
| 1   | AA    | 1370 | G    |
| 1   | AA    | 1371 | G    |
| 1   | AA    | 1372 | U    |
| 1   | AA    | 1373 | G    |
| 1   | AA    | 1385 | G    |
| 1   | AA    | 1386 | G    |
| 1   | AA    | 1387 | G    |
| 1   | AA    | 1390 | U    |
| 1   | AA    | 1391 | U    |
| 1   | AA    | 1398 | A    |
| 1   | AA    | 1399 | C    |
| 1   | AA    | 1400 | C    |
| 1   | AA    | 1401 | G    |
| 1   | AA    | 1402 | C    |
| 1   | AA    | 1408 | A    |
| 1   | AA    | 1419 | G    |
| 1   | AA    | 1442 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 1442(A) | G    |
| 1   | AA    | 1446    | U    |
| 1   | AA    | 1447    | A    |
| 1   | AA    | 1452    | C    |
| 1   | AA    | 1456    | G    |
| 1   | AA    | 1457    | G    |
| 1   | AA    | 1487    | G    |
| 1   | AA    | 1490    | C    |
| 1   | AA    | 1491    | G    |
| 1   | AA    | 1492    | A    |
| 1   | AA    | 1493    | A    |
| 1   | AA    | 1499    | A    |
| 1   | AA    | 1503    | A    |
| 1   | AA    | 1504    | G    |
| 1   | AA    | 1505    | G    |
| 1   | AA    | 1506    | U    |
| 1   | AA    | 1507    | A    |
| 1   | AA    | 1517    | G    |
| 1   | AA    | 1520    | G    |
| 1   | AA    | 1524    | C    |
| 1   | AA    | 1525    | G    |
| 1   | AA    | 1526    | G    |
| 1   | AA    | 1529    | G    |
| 1   | AA    | 1530    | G    |
| 1   | AA    | 1533    | C    |
| 22  | AV    | 10      | G    |
| 22  | AV    | 13      | C    |
| 22  | AV    | 15      | G    |
| 22  | AV    | 16      | C    |
| 22  | AV    | 17      | C    |
| 22  | AV    | 18      | G    |
| 22  | AV    | 19      | G    |
| 22  | AV    | 20      | U    |
| 22  | AV    | 21      | A    |
| 22  | AV    | 22      | G    |
| 22  | AV    | 23      | A    |
| 22  | AV    | 30      | G    |
| 22  | AV    | 34      | G    |
| 22  | AV    | 44      | G    |
| 22  | AV    | 45      | U    |
| 22  | AV    | 46      | G    |
| 22  | AV    | 48      | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | AV    | 52  | G    |
| 22  | AV    | 53  | G    |
| 22  | AV    | 61  | C    |
| 22  | AV    | 73  | A    |
| 22  | AV    | 74  | C    |
| 22  | AV    | 75  | C    |
| 22  | AV    | 76  | A    |
| 23  | AX    | 12  | A    |
| 23  | AX    | 13  | A    |
| 23  | AX    | 19  | A    |
| 35  | BA    | 9   | U    |
| 35  | BA    | 10  | G    |
| 35  | BA    | 16  | G    |
| 35  | BA    | 28  | A    |
| 35  | BA    | 29  | U    |
| 35  | BA    | 30  | G    |
| 35  | BA    | 32  | C    |
| 35  | BA    | 34  | C    |
| 35  | BA    | 36  | G    |
| 35  | BA    | 37  | C    |
| 35  | BA    | 44  | G    |
| 35  | BA    | 45  | C    |
| 35  | BA    | 49  | A    |
| 35  | BA    | 50  | U    |
| 35  | BA    | 53  | A    |
| 35  | BA    | 58  | G    |
| 35  | BA    | 71  | A    |
| 35  | BA    | 72  | U    |
| 35  | BA    | 74  | A    |
| 35  | BA    | 75  | G    |
| 35  | BA    | 83  | G    |
| 35  | BA    | 84  | A    |
| 35  | BA    | 88  | G    |
| 35  | BA    | 90  | U    |
| 35  | BA    | 94  | C    |
| 35  | BA    | 102 | G    |
| 35  | BA    | 109 | G    |
| 35  | BA    | 110 | G    |
| 35  | BA    | 111 | A    |
| 35  | BA    | 112 | U    |
| 35  | BA    | 115 | C    |
| 35  | BA    | 118 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | BA    | 119    | A    |
| 35  | BA    | 120    | U    |
| 35  | BA    | 139(A) | G    |
| 35  | BA    | 140    | G    |
| 35  | BA    | 141    | A    |
| 35  | BA    | 146    | G    |
| 35  | BA    | 174    | C    |
| 35  | BA    | 175    | G    |
| 35  | BA    | 177    | G    |
| 35  | BA    | 178    | G    |
| 35  | BA    | 179    | G    |
| 35  | BA    | 180    | G    |
| 35  | BA    | 181    | A    |
| 35  | BA    | 182    | A    |
| 35  | BA    | 196    | A    |
| 35  | BA    | 197    | A    |
| 35  | BA    | 199    | A    |
| 35  | BA    | 205    | G    |
| 35  | BA    | 215    | G    |
| 35  | BA    | 216    | A    |
| 35  | BA    | 221    | A    |
| 35  | BA    | 222    | A    |
| 35  | BA    | 228    | A    |
| 35  | BA    | 229    | A    |
| 35  | BA    | 230    | U    |
| 35  | BA    | 233    | A    |
| 35  | BA    | 247    | G    |
| 35  | BA    | 248    | G    |
| 35  | BA    | 249    | C    |
| 35  | BA    | 252    | G    |
| 35  | BA    | 257    | A    |
| 35  | BA    | 262    | A    |
| 35  | BA    | 264    | C    |
| 35  | BA    | 265    | A    |
| 35  | BA    | 266    | G    |
| 35  | BA    | 271(I) | G    |
| 35  | BA    | 271(J) | C    |
| 35  | BA    | 271(K) | U    |
| 35  | BA    | 271(M) | G    |
| 35  | BA    | 271(N) | U    |
| 35  | BA    | 271(O) | C    |
| 35  | BA    | 271(P) | C    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 271(R)     | G           |
| 35         | BA           | 271(Y)     | U           |
| 35         | BA           | 272(A)     | U           |
| 35         | BA           | 272(B)     | G           |
| 35         | BA           | 272(I)     | U           |
| 35         | BA           | 274        | G           |
| 35         | BA           | 275        | G           |
| 35         | BA           | 276        | A           |
| 35         | BA           | 277        | C           |
| 35         | BA           | 311        | A           |
| 35         | BA           | 329        | G           |
| 35         | BA           | 330        | A           |
| 35         | BA           | 331        | A           |
| 35         | BA           | 332        | A           |
| 35         | BA           | 333        | G           |
| 35         | BA           | 334        | C           |
| 35         | BA           | 352        | G           |
| 35         | BA           | 353        | G           |
| 35         | BA           | 356        | G           |
| 35         | BA           | 362        | U           |
| 35         | BA           | 363(E)     | U           |
| 35         | BA           | 364        | C           |
| 35         | BA           | 386        | G           |
| 35         | BA           | 387        | U           |
| 35         | BA           | 388        | G           |
| 35         | BA           | 396        | G           |
| 35         | BA           | 405        | U           |
| 35         | BA           | 411        | G           |
| 35         | BA           | 412        | A           |
| 35         | BA           | 418        | G           |
| 35         | BA           | 428        | A           |
| 35         | BA           | 444        | C           |
| 35         | BA           | 448        | U           |
| 35         | BA           | 454        | A           |
| 35         | BA           | 456        | C           |
| 35         | BA           | 457        | A           |
| 35         | BA           | 460        | A           |
| 35         | BA           | 462        | C           |
| 35         | BA           | 463        | G           |
| 35         | BA           | 464        | U           |
| 35         | BA           | 467        | G           |
| 35         | BA           | 470        | A           |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | BA    | 473    | G    |
| 35  | BA    | 481    | G    |
| 35  | BA    | 505    | A    |
| 35  | BA    | 508    | G    |
| 35  | BA    | 509    | C    |
| 35  | BA    | 525    | U    |
| 35  | BA    | 526    | A    |
| 35  | BA    | 527    | C    |
| 35  | BA    | 528    | A    |
| 35  | BA    | 530    | G    |
| 35  | BA    | 531    | C    |
| 35  | BA    | 532    | A    |
| 35  | BA    | 533    | G    |
| 35  | BA    | 563    | G    |
| 35  | BA    | 573    | G    |
| 35  | BA    | 575    | A    |
| 35  | BA    | 586    | A    |
| 35  | BA    | 588    | U    |
| 35  | BA    | 600    | G    |
| 35  | BA    | 603    | A    |
| 35  | BA    | 604    | G    |
| 35  | BA    | 605    | C    |
| 35  | BA    | 607    | U    |
| 35  | BA    | 613    | G    |
| 35  | BA    | 614(B) | G    |
| 35  | BA    | 627    | A    |
| 35  | BA    | 628    | G    |
| 35  | BA    | 629    | G    |
| 35  | BA    | 630    | G    |
| 35  | BA    | 637    | A    |
| 35  | BA    | 645    | C    |
| 35  | BA    | 646    | A    |
| 35  | BA    | 651    | G    |
| 35  | BA    | 653    | A    |
| 35  | BA    | 654    | A    |
| 35  | BA    | 654(I) | C    |
| 35  | BA    | 654(J) | A    |
| 35  | BA    | 654(K) | C    |
| 35  | BA    | 654(T) | C    |
| 35  | BA    | 655    | A    |
| 35  | BA    | 656    | G    |
| 35  | BA    | 686    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BA    | 689 | A    |
| 35  | BA    | 690 | G    |
| 35  | BA    | 691 | C    |
| 35  | BA    | 692 | C    |
| 35  | BA    | 693 | C    |
| 35  | BA    | 697 | C    |
| 35  | BA    | 698 | C    |
| 35  | BA    | 699 | A    |
| 35  | BA    | 708 | C    |
| 35  | BA    | 722 | A    |
| 35  | BA    | 730 | C    |
| 35  | BA    | 740 | U    |
| 35  | BA    | 742 | G    |
| 35  | BA    | 743 | G    |
| 35  | BA    | 744 | G    |
| 35  | BA    | 753 | C    |
| 35  | BA    | 764 | A    |
| 35  | BA    | 776 | G    |
| 35  | BA    | 782 | A    |
| 35  | BA    | 784 | A    |
| 35  | BA    | 785 | G    |
| 35  | BA    | 790 | C    |
| 35  | BA    | 791 | C    |
| 35  | BA    | 792 | G    |
| 35  | BA    | 805 | G    |
| 35  | BA    | 812 | C    |
| 35  | BA    | 819 | A    |
| 35  | BA    | 827 | U    |
| 35  | BA    | 828 | U    |
| 35  | BA    | 830 | G    |
| 35  | BA    | 848 | G    |
| 35  | BA    | 856 | C    |
| 35  | BA    | 857 | C    |
| 35  | BA    | 858 | U    |
| 35  | BA    | 859 | G    |
| 35  | BA    | 860 | U    |
| 35  | BA    | 866 | A    |
| 35  | BA    | 878 | A    |
| 35  | BA    | 881 | G    |
| 35  | BA    | 885 | C    |
| 35  | BA    | 886 | C    |
| 35  | BA    | 887 | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 888        | C           |
| 35         | BA           | 889        | C           |
| 35         | BA           | 890        | A           |
| 35         | BA           | 892        | G           |
| 35         | BA           | 893        | C           |
| 35         | BA           | 896        | A           |
| 35         | BA           | 897        | C           |
| 35         | BA           | 901        | A           |
| 35         | BA           | 910        | A           |
| 35         | BA           | 917        | A           |
| 35         | BA           | 926        | A           |
| 35         | BA           | 932        | G           |
| 35         | BA           | 934        | G           |
| 35         | BA           | 941        | A           |
| 35         | BA           | 945        | A           |
| 35         | BA           | 946        | G           |
| 35         | BA           | 954        | G           |
| 35         | BA           | 955        | C           |
| 35         | BA           | 956        | G           |
| 35         | BA           | 958        | U           |
| 35         | BA           | 959        | A           |
| 35         | BA           | 961        | C           |
| 35         | BA           | 966        | G           |
| 35         | BA           | 968        | G           |
| 35         | BA           | 970        | C           |
| 35         | BA           | 974        | G           |
| 35         | BA           | 975        | C           |
| 35         | BA           | 983        | A           |
| 35         | BA           | 996        | A           |
| 35         | BA           | 1011       | G           |
| 35         | BA           | 1012       | U           |
| 35         | BA           | 1013       | C           |
| 35         | BA           | 1016       | G           |
| 35         | BA           | 1023       | U           |
| 35         | BA           | 1026       | U           |
| 35         | BA           | 1027       | A           |
| 35         | BA           | 1033       | U           |
| 35         | BA           | 1039       | G           |
| 35         | BA           | 1045       | A           |
| 35         | BA           | 1046       | A           |
| 35         | BA           | 1047       | G           |
| 35         | BA           | 1048       | A           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | BA    | 1059    | G    |
| 35  | BA    | 1061    | U    |
| 35  | BA    | 1065    | U    |
| 35  | BA    | 1066    | U    |
| 35  | BA    | 1067    | A    |
| 35  | BA    | 1068    | G    |
| 35  | BA    | 1069    | A    |
| 35  | BA    | 1070    | A    |
| 35  | BA    | 1073    | A    |
| 35  | BA    | 1074    | G    |
| 35  | BA    | 1087    | G    |
| 35  | BA    | 1088    | A    |
| 35  | BA    | 1091    | G    |
| 35  | BA    | 1101    | U    |
| 35  | BA    | 1105    | U    |
| 35  | BA    | 1106    | G    |
| 35  | BA    | 1110    | G    |
| 35  | BA    | 1111    | A    |
| 35  | BA    | 1112    | G    |
| 35  | BA    | 1114    | G    |
| 35  | BA    | 1116    | C    |
| 35  | BA    | 1119    | C    |
| 35  | BA    | 1120    | G    |
| 35  | BA    | 1130    | U    |
| 35  | BA    | 1133    | U    |
| 35  | BA    | 1136    | G    |
| 35  | BA    | 1137    | G    |
| 35  | BA    | 1142    | U    |
| 35  | BA    | 1142(A) | A    |
| 35  | BA    | 1155    | A    |
| 35  | BA    | 1173    | G    |
| 35  | BA    | 1174    | A    |
| 35  | BA    | 1175    | U    |
| 35  | BA    | 1176    | G    |
| 35  | BA    | 1178    | C    |
| 35  | BA    | 1180    | C    |
| 35  | BA    | 1205    | U    |
| 35  | BA    | 1210    | A    |
| 35  | BA    | 1211    | U    |
| 35  | BA    | 1213    | A    |
| 35  | BA    | 1220    | A    |
| 35  | BA    | 1221    | C    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1223       | G           |
| 35         | BA           | 1224       | C           |
| 35         | BA           | 1253       | A           |
| 35         | BA           | 1256       | G           |
| 35         | BA           | 1265       | A           |
| 35         | BA           | 1271       | G           |
| 35         | BA           | 1272       | A           |
| 35         | BA           | 1273       | U           |
| 35         | BA           | 1284       | A           |
| 35         | BA           | 1285       | G           |
| 35         | BA           | 1287       | A           |
| 35         | BA           | 1300       | U           |
| 35         | BA           | 1301       | A           |
| 35         | BA           | 1302       | A           |
| 35         | BA           | 1314       | C           |
| 35         | BA           | 1319       | G           |
| 35         | BA           | 1321       | A           |
| 35         | BA           | 1332       | G           |
| 35         | BA           | 1345       | C           |
| 35         | BA           | 1349       | A           |
| 35         | BA           | 1359       | A           |
| 35         | BA           | 1365       | A           |
| 35         | BA           | 1368       | G           |
| 35         | BA           | 1377       | G           |
| 35         | BA           | 1378       | A           |
| 35         | BA           | 1380       | G           |
| 35         | BA           | 1382       | G           |
| 35         | BA           | 1384       | A           |
| 35         | BA           | 1385       | G           |
| 35         | BA           | 1386       | C           |
| 35         | BA           | 1396       | U           |
| 35         | BA           | 1407       | C           |
| 35         | BA           | 1416       | G           |
| 35         | BA           | 1417       | C           |
| 35         | BA           | 1420       | U           |
| 35         | BA           | 1425       | G           |
| 35         | BA           | 1426       | G           |
| 35         | BA           | 1427       | A           |
| 35         | BA           | 1428       | C           |
| 35         | BA           | 1437       | C           |
| 35         | BA           | 1445       | A           |
| 35         | BA           | 1449       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1450       | G           |
| 35         | BA           | 1456       | G           |
| 35         | BA           | 1459       | G           |
| 35         | BA           | 1460       | A           |
| 35         | BA           | 1461       | G           |
| 35         | BA           | 1462       | C           |
| 35         | BA           | 1467       | C           |
| 35         | BA           | 1471       | A           |
| 35         | BA           | 1475       | G           |
| 35         | BA           | 1478       | G           |
| 35         | BA           | 1482       | G           |
| 35         | BA           | 1485       | G           |
| 35         | BA           | 1490       | A           |
| 35         | BA           | 1493       | C           |
| 35         | BA           | 1494       | A           |
| 35         | BA           | 1495       | A           |
| 35         | BA           | 1497       | U           |
| 35         | BA           | 1501       | C           |
| 35         | BA           | 1502       | C           |
| 35         | BA           | 1505       | C           |
| 35         | BA           | 1509       | C           |
| 35         | BA           | 1509(A)    | A           |
| 35         | BA           | 1517       | G           |
| 35         | BA           | 1534       | U           |
| 35         | BA           | 1541       | G           |
| 35         | BA           | 1542       | A           |
| 35         | BA           | 1543       | C           |
| 35         | BA           | 1544       | A           |
| 35         | BA           | 1547       | C           |
| 35         | BA           | 1554       | A           |
| 35         | BA           | 1558       | A           |
| 35         | BA           | 1559       | G           |
| 35         | BA           | 1569       | A           |
| 35         | BA           | 1578       | U           |
| 35         | BA           | 1579       | A           |
| 35         | BA           | 1581       | G           |
| 35         | BA           | 1584       | C           |
| 35         | BA           | 1586       | A           |
| 35         | BA           | 1588       | C           |
| 35         | BA           | 1591       | G           |
| 35         | BA           | 1597       | A           |
| 35         | BA           | 1598       | C           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | BA    | 1599    | C    |
| 35  | BA    | 1608    | A    |
| 35  | BA    | 1616    | A    |
| 35  | BA    | 1617    | C    |
| 35  | BA    | 1618    | A    |
| 35  | BA    | 1639    | U    |
| 35  | BA    | 1640    | C    |
| 35  | BA    | 1642    | G    |
| 35  | BA    | 1643    | G    |
| 35  | BA    | 1646    | C    |
| 35  | BA    | 1647    | G    |
| 35  | BA    | 1648    | C    |
| 35  | BA    | 1653    | G    |
| 35  | BA    | 1654    | A    |
| 35  | BA    | 1674    | G    |
| 35  | BA    | 1696    | G    |
| 35  | BA    | 1698    | A    |
| 35  | BA    | 1699    | G    |
| 35  | BA    | 1702    | G    |
| 35  | BA    | 1718    | G    |
| 35  | BA    | 1721    | G    |
| 35  | BA    | 1722    | A    |
| 35  | BA    | 1739    | U    |
| 35  | BA    | 1740    | G    |
| 35  | BA    | 1741    | A    |
| 35  | BA    | 1745(A) | C    |
| 35  | BA    | 1746    | G    |
| 35  | BA    | 1748    | G    |
| 35  | BA    | 1750    | G    |
| 35  | BA    | 1763    | G    |
| 35  | BA    | 1764    | G    |
| 35  | BA    | 1768    | U    |
| 35  | BA    | 1770    | G    |
| 35  | BA    | 1772    | G    |
| 35  | BA    | 1773    | A    |
| 35  | BA    | 1776    | G    |
| 35  | BA    | 1779    | U    |
| 35  | BA    | 1780    | A    |
| 35  | BA    | 1781    | C    |
| 35  | BA    | 1782    | C    |
| 35  | BA    | 1786    | A    |
| 35  | BA    | 1787    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1788       | C           |
| 35         | BA           | 1791       | A           |
| 35         | BA           | 1799       | G           |
| 35         | BA           | 1800       | C           |
| 35         | BA           | 1801       | G           |
| 35         | BA           | 1805       | U           |
| 35         | BA           | 1806       | C           |
| 35         | BA           | 1808       | U           |
| 35         | BA           | 1816       | G           |
| 35         | BA           | 1820       | U           |
| 35         | BA           | 1821       | A           |
| 35         | BA           | 1822       | G           |
| 35         | BA           | 1829       | A           |
| 35         | BA           | 1835       | G           |
| 35         | BA           | 1839       | G           |
| 35         | BA           | 1847       | A           |
| 35         | BA           | 1848       | A           |
| 35         | BA           | 1858       | G           |
| 35         | BA           | 1865       | G           |
| 35         | BA           | 1877       | A           |
| 35         | BA           | 1878       | G           |
| 35         | BA           | 1881       | C           |
| 35         | BA           | 1885       | A           |
| 35         | BA           | 1888       | G           |
| 35         | BA           | 1889       | A           |
| 35         | BA           | 1890       | A           |
| 35         | BA           | 1891       | G           |
| 35         | BA           | 1893       | C           |
| 35         | BA           | 1906       | G           |
| 35         | BA           | 1907       | G           |
| 35         | BA           | 1912       | A           |
| 35         | BA           | 1913       | A           |
| 35         | BA           | 1914       | C           |
| 35         | BA           | 1920       | C           |
| 35         | BA           | 1925       | C           |
| 35         | BA           | 1926       | U           |
| 35         | BA           | 1930       | G           |
| 35         | BA           | 1936       | A           |
| 35         | BA           | 1937       | A           |
| 35         | BA           | 1938       | A           |
| 35         | BA           | 1941       | C           |
| 35         | BA           | 1955       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1962       | C           |
| 35         | BA           | 1963       | U           |
| 35         | BA           | 1965       | C           |
| 35         | BA           | 1967       | C           |
| 35         | BA           | 1969       | A           |
| 35         | BA           | 1970       | A           |
| 35         | BA           | 1971       | A           |
| 35         | BA           | 1972       | A           |
| 35         | BA           | 1982       | C           |
| 35         | BA           | 1984       | G           |
| 35         | BA           | 1985       | G           |
| 35         | BA           | 1987       | G           |
| 35         | BA           | 1988       | C           |
| 35         | BA           | 1989       | G           |
| 35         | BA           | 1992       | G           |
| 35         | BA           | 1993       | U           |
| 35         | BA           | 1995       | U           |
| 35         | BA           | 1996       | C           |
| 35         | BA           | 1997       | G           |
| 35         | BA           | 1998       | G           |
| 35         | BA           | 2000       | G           |
| 35         | BA           | 2010       | G           |
| 35         | BA           | 2011       | U           |
| 35         | BA           | 2020       | A           |
| 35         | BA           | 2023       | G           |
| 35         | BA           | 2027       | G           |
| 35         | BA           | 2031       | A           |
| 35         | BA           | 2032       | G           |
| 35         | BA           | 2033       | A           |
| 35         | BA           | 2034       | U           |
| 35         | BA           | 2036       | C           |
| 35         | BA           | 2043       | C           |
| 35         | BA           | 2051       | A           |
| 35         | BA           | 2055       | C           |
| 35         | BA           | 2056       | G           |
| 35         | BA           | 2060       | A           |
| 35         | BA           | 2061       | G           |
| 35         | BA           | 2062       | A           |
| 35         | BA           | 2069       | G           |
| 35         | BA           | 2099       | U           |
| 35         | BA           | 2100       | G           |
| 35         | BA           | 2103       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 2104       | G           |
| 35         | BA           | 2105       | C           |
| 35         | BA           | 2106       | G           |
| 35         | BA           | 2110       | G           |
| 35         | BA           | 2111       | C           |
| 35         | BA           | 2112       | G           |
| 35         | BA           | 2116       | G           |
| 35         | BA           | 2117       | A           |
| 35         | BA           | 2118       | U           |
| 35         | BA           | 2127       | G           |
| 35         | BA           | 2128       | C           |
| 35         | BA           | 2129       | C           |
| 35         | BA           | 2132       | U           |
| 35         | BA           | 2133       | A           |
| 35         | BA           | 2134       | A           |
| 35         | BA           | 2137       | C           |
| 35         | BA           | 2138       | C           |
| 35         | BA           | 2140       | C           |
| 35         | BA           | 2145       | C           |
| 35         | BA           | 2146       | C           |
| 35         | BA           | 2147       | G           |
| 35         | BA           | 2152       | G           |
| 35         | BA           | 2153       | G           |
| 35         | BA           | 2154       | G           |
| 35         | BA           | 2158       | A           |
| 35         | BA           | 2159       | G           |
| 35         | BA           | 2172       | U           |
| 35         | BA           | 2173       | A           |
| 35         | BA           | 2174       | C           |
| 35         | BA           | 2175       | C           |
| 35         | BA           | 2177       | C           |
| 35         | BA           | 2178       | C           |
| 35         | BA           | 2180       | U           |
| 35         | BA           | 2186       | G           |
| 35         | BA           | 2187       | G           |
| 35         | BA           | 2190       | G           |
| 35         | BA           | 2193       | G           |
| 35         | BA           | 2198       | A           |
| 35         | BA           | 2199       | A           |
| 35         | BA           | 2200       | C           |
| 35         | BA           | 2201       | C           |
| 35         | BA           | 2202       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 2206       | G           |
| 35         | BA           | 2207       | G           |
| 35         | BA           | 2208       | A           |
| 35         | BA           | 2218       | U           |
| 35         | BA           | 2219       | G           |
| 35         | BA           | 2225       | A           |
| 35         | BA           | 2238       | G           |
| 35         | BA           | 2239       | G           |
| 35         | BA           | 2275       | C           |
| 35         | BA           | 2283       | C           |
| 35         | BA           | 2287       | A           |
| 35         | BA           | 2288       | A           |
| 35         | BA           | 2305       | A           |
| 35         | BA           | 2307       | G           |
| 35         | BA           | 2308       | G           |
| 35         | BA           | 2309       | A           |
| 35         | BA           | 2313       | C           |
| 35         | BA           | 2316       | C           |
| 35         | BA           | 2319       | G           |
| 35         | BA           | 2320       | A           |
| 35         | BA           | 2334       | G           |
| 35         | BA           | 2336       | A           |
| 35         | BA           | 2347       | C           |
| 35         | BA           | 2350       | C           |
| 35         | BA           | 2356       | C           |
| 35         | BA           | 2357       | U           |
| 35         | BA           | 2361       | A           |
| 35         | BA           | 2364       | C           |
| 35         | BA           | 2383       | G           |
| 35         | BA           | 2385       | C           |
| 35         | BA           | 2392       | A           |
| 35         | BA           | 2400       | G           |
| 35         | BA           | 2401       | U           |
| 35         | BA           | 2402       | C           |
| 35         | BA           | 2403       | C           |
| 35         | BA           | 2404       | C           |
| 35         | BA           | 2405       | G           |
| 35         | BA           | 2406       | U           |
| 35         | BA           | 2409       | G           |
| 35         | BA           | 2423       | U           |
| 35         | BA           | 2425       | A           |
| 35         | BA           | 2429       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 2430       | A           |
| 35         | BA           | 2431       | U           |
| 35         | BA           | 2439       | A           |
| 35         | BA           | 2441       | C           |
| 35         | BA           | 2447       | G           |
| 35         | BA           | 2448       | A           |
| 35         | BA           | 2465       | C           |
| 35         | BA           | 2469       | A           |
| 35         | BA           | 2470       | G           |
| 35         | BA           | 2476       | A           |
| 35         | BA           | 2482       | G           |
| 35         | BA           | 2484       | G           |
| 35         | BA           | 2491       | U           |
| 35         | BA           | 2502       | G           |
| 35         | BA           | 2505       | G           |
| 35         | BA           | 2518       | A           |
| 35         | BA           | 2524       | G           |
| 35         | BA           | 2529       | G           |
| 35         | BA           | 2542       | A           |
| 35         | BA           | 2543       | G           |
| 35         | BA           | 2552       | U           |
| 35         | BA           | 2554       | U           |
| 35         | BA           | 2555       | U           |
| 35         | BA           | 2556       | C           |
| 35         | BA           | 2557       | G           |
| 35         | BA           | 2558       | C           |
| 35         | BA           | 2560       | C           |
| 35         | BA           | 2566       | A           |
| 35         | BA           | 2567       | G           |
| 35         | BA           | 2573       | C           |
| 35         | BA           | 2578       | G           |
| 35         | BA           | 2586       | C           |
| 35         | BA           | 2602       | A           |
| 35         | BA           | 2603       | G           |
| 35         | BA           | 2607       | G           |
| 35         | BA           | 2608       | G           |
| 35         | BA           | 2609       | U           |
| 35         | BA           | 2610       | C           |
| 35         | BA           | 2611       | U           |
| 35         | BA           | 2612       | C           |
| 35         | BA           | 2613       | U           |
| 35         | BA           | 2615       | U           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | BA    | 2630    | G    |
| 35  | BA    | 2654    | A    |
| 35  | BA    | 2657    | A    |
| 35  | BA    | 2658    | C    |
| 35  | BA    | 2673    | G    |
| 35  | BA    | 2690    | C    |
| 35  | BA    | 2691    | C    |
| 35  | BA    | 2712    | U    |
| 35  | BA    | 2712(A) | A    |
| 35  | BA    | 2713    | A    |
| 35  | BA    | 2714    | G    |
| 35  | BA    | 2717    | G    |
| 35  | BA    | 2726    | U    |
| 35  | BA    | 2733    | A    |
| 35  | BA    | 2750    | A    |
| 35  | BA    | 2751    | G    |
| 35  | BA    | 2752    | C    |
| 35  | BA    | 2753    | A    |
| 35  | BA    | 2756    | U    |
| 35  | BA    | 2757    | A    |
| 35  | BA    | 2758    | A    |
| 35  | BA    | 2759    | G    |
| 35  | BA    | 2764    | A    |
| 35  | BA    | 2765    | A    |
| 35  | BA    | 2766    | G    |
| 35  | BA    | 2778    | A    |
| 35  | BA    | 2779    | U    |
| 35  | BA    | 2780    | G    |
| 35  | BA    | 2789    | C    |
| 35  | BA    | 2790    | A    |
| 35  | BA    | 2791    | C    |
| 35  | BA    | 2794    | C    |
| 35  | BA    | 2799    | C    |
| 35  | BA    | 2802    | G    |
| 35  | BA    | 2803    | C    |
| 35  | BA    | 2808    | U    |
| 35  | BA    | 2820    | A    |
| 35  | BA    | 2821    | A    |
| 35  | BA    | 2833    | G    |
| 35  | BA    | 2834    | G    |
| 35  | BA    | 2835    | A    |
| 35  | BA    | 2849    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BA    | 2872 | G    |
| 35  | BA    | 2893 | G    |
| 35  | BA    | 2894 | G    |
| 36  | BB    | 8    | U    |
| 36  | BB    | 13   | A    |
| 36  | BB    | 15   | A    |
| 36  | BB    | 17   | C    |
| 36  | BB    | 21   | G    |
| 36  | BB    | 25   | A    |
| 36  | BB    | 26   | A    |
| 36  | BB    | 27   | C    |
| 36  | BB    | 32   | C    |
| 36  | BB    | 35   | U    |
| 36  | BB    | 39   | A    |
| 36  | BB    | 40   | U    |
| 36  | BB    | 41   | U    |
| 36  | BB    | 42   | C    |
| 36  | BB    | 43   | C    |
| 36  | BB    | 45   | A    |
| 36  | BB    | 53   | A    |
| 36  | BB    | 57   | A    |
| 36  | BB    | 66   | A    |
| 36  | BB    | 67   | G    |
| 36  | BB    | 68   | C    |
| 36  | BB    | 73   | A    |
| 36  | BB    | 81   | G    |
| 36  | BB    | 88   | C    |
| 36  | BB    | 110  | G    |
| 36  | BB    | 113  | G    |

All (115) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 60  | A    |
| 1   | AA    | 64  | G    |
| 1   | AA    | 78  | G    |
| 1   | AA    | 84  | U    |
| 1   | AA    | 89  | C    |
| 1   | AA    | 90  | U    |
| 1   | AA    | 115 | G    |
| 1   | AA    | 119 | A    |
| 1   | AA    | 197 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 243     | A    |
| 1   | AA    | 250     | A    |
| 1   | AA    | 266     | G    |
| 1   | AA    | 274     | A    |
| 1   | AA    | 344     | A    |
| 1   | AA    | 353     | A    |
| 1   | AA    | 388     | G    |
| 1   | AA    | 412     | A    |
| 1   | AA    | 428     | G    |
| 1   | AA    | 429     | U    |
| 1   | AA    | 484     | G    |
| 1   | AA    | 495     | A    |
| 1   | AA    | 547     | A    |
| 1   | AA    | 560     | U    |
| 1   | AA    | 573     | A    |
| 1   | AA    | 575     | G    |
| 1   | AA    | 687     | A    |
| 1   | AA    | 748     | C    |
| 1   | AA    | 792     | A    |
| 1   | AA    | 968     | A    |
| 1   | AA    | 980     | C    |
| 1   | AA    | 982     | U    |
| 1   | AA    | 992     | U    |
| 1   | AA    | 1003    | G    |
| 1   | AA    | 1030(D) | A    |
| 1   | AA    | 1049    | U    |
| 1   | AA    | 1053    | G    |
| 1   | AA    | 1101    | A    |
| 1   | AA    | 1139    | G    |
| 1   | AA    | 1157    | A    |
| 1   | AA    | 1200    | C    |
| 1   | AA    | 1229    | A    |
| 1   | AA    | 1239    | A    |
| 1   | AA    | 1279    | A    |
| 1   | AA    | 1285    | A    |
| 1   | AA    | 1399    | C    |
| 1   | AA    | 1447    | A    |
| 1   | AA    | 1452    | C    |
| 1   | AA    | 1456    | G    |
| 1   | AA    | 1492    | A    |
| 1   | AA    | 1498    | U    |
| 1   | AA    | 1504    | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 22         | AV           | 15         | G           |
| 22         | AV           | 16         | C           |
| 35         | BA           | 49         | A           |
| 35         | BA           | 71         | A           |
| 35         | BA           | 74         | A           |
| 35         | BA           | 197        | A           |
| 35         | BA           | 221        | A           |
| 35         | BA           | 331        | A           |
| 35         | BA           | 332        | A           |
| 35         | BA           | 363(F)     | A           |
| 35         | BA           | 387        | U           |
| 35         | BA           | 587        | C           |
| 35         | BA           | 603        | A           |
| 35         | BA           | 627        | A           |
| 35         | BA           | 752        | A           |
| 35         | BA           | 764        | A           |
| 35         | BA           | 790        | C           |
| 35         | BA           | 856        | C           |
| 35         | BA           | 887        | A           |
| 35         | BA           | 974        | G           |
| 35         | BA           | 1060       | U           |
| 35         | BA           | 1068       | G           |
| 35         | BA           | 1210       | A           |
| 35         | BA           | 1300       | U           |
| 35         | BA           | 1301       | A           |
| 35         | BA           | 1379       | A           |
| 35         | BA           | 1427       | A           |
| 35         | BA           | 1540       | U           |
| 35         | BA           | 1541       | G           |
| 35         | BA           | 1558       | A           |
| 35         | BA           | 1591       | G           |
| 35         | BA           | 1608       | A           |
| 35         | BA           | 1653       | G           |
| 35         | BA           | 1799       | G           |
| 35         | BA           | 1819       | A           |
| 35         | BA           | 1820       | U           |
| 35         | BA           | 1839       | G           |
| 35         | BA           | 1992       | G           |
| 35         | BA           | 2033       | A           |
| 35         | BA           | 2103       | C           |
| 35         | BA           | 2104       | G           |
| 35         | BA           | 2111       | C           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BA    | 2116 | G    |
| 35  | BA    | 2117 | A    |
| 35  | BA    | 2126 | A    |
| 35  | BA    | 2136 | C    |
| 35  | BA    | 2137 | C    |
| 35  | BA    | 2145 | C    |
| 35  | BA    | 2157 | G    |
| 35  | BA    | 2176 | A    |
| 35  | BA    | 2180 | U    |
| 35  | BA    | 2282 | G    |
| 35  | BA    | 2401 | U    |
| 35  | BA    | 2402 | C    |
| 35  | BA    | 2422 | A    |
| 35  | BA    | 2439 | A    |
| 35  | BA    | 2481 | G    |
| 35  | BA    | 2542 | A    |
| 35  | BA    | 2610 | C    |
| 35  | BA    | 2689 | U    |
| 35  | BA    | 2750 | A    |
| 35  | BA    | 2756 | U    |
| 36  | BB    | 56   | G    |
| 36  | BB    | 66   | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 527 ligands modelled in this entry, 526 are monoatomic - leaving 1 for Mogul analysis.

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 61  | GCP  | AY    | 701 | 59   | 25,34,34     | 3.54 | 8 (32%)     | 28,54,54    | 1.58 | 7 (25%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 61  | GCP  | AY    | 701 | 59   | -       | 0/18/38/38 | 0/3/3/3 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 61  | AY    | 701 | GCP  | C5-C6  | -10.79 | 1.33        | 1.53     |
| 61  | AY    | 701 | GCP  | C4-N9  | -10.76 | 1.33        | 1.47     |
| 61  | AY    | 701 | GCP  | C8-N9  | -4.41  | 1.33        | 1.46     |
| 61  | AY    | 701 | GCP  | PB-O2B | -3.32  | 1.48        | 1.56     |
| 61  | AY    | 701 | GCP  | PG-O3G | -3.24  | 1.47        | 1.54     |
| 61  | AY    | 701 | GCP  | PG-O2G | -2.76  | 1.48        | 1.54     |
| 61  | AY    | 701 | GCP  | PB-O3A | 2.45   | 1.61        | 1.58     |
| 61  | AY    | 701 | GCP  | C6-N1  | 4.14   | 1.40        | 1.33     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 61  | AY    | 701 | GCP  | PA-O3A-PB   | -3.85 | 119.98      | 132.39   |
| 61  | AY    | 701 | GCP  | O1G-PG-C3B  | -3.27 | 104.02      | 111.22   |
| 61  | AY    | 701 | GCP  | C4'-O4'-C1' | -2.47 | 103.96      | 109.47   |
| 61  | AY    | 701 | GCP  | O6-C6-N1    | -2.31 | 119.62      | 122.70   |
| 61  | AY    | 701 | GCP  | O2G-PG-C3B  | -2.23 | 101.00      | 106.40   |
| 61  | AY    | 701 | GCP  | O3G-PG-O2G  | 2.15  | 114.44      | 108.14   |
| 61  | AY    | 701 | GCP  | O2B-PB-O1B  | 2.85  | 119.61      | 110.09   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:



| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 61  | AY    | 701 | GCP  | 11      | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 35  | BA    | 3                |
| 1   | AA    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | AA    | 496:A     | O3'    | 498:U     | P      | 3.07         |
| 1     | BA    | 45:C      | O3'    | 47:C      | P      | 2.97         |
| 1     | BA    | 1133:U    | O3'    | 1135:C    | P      | 2.48         |
| 1     | BA    | 2203:U    | O3'    | 2205:C    | P      | 2.42         |

## 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    | 1507/1519 (99%) | 0.18   | 52 (3%) 44 28 | 24, 47, 125, 239      | 0     |
| 2   | AB    | 235/256 (91%)   | 0.47   | 19 (8%) 13 7  | 34, 61, 112, 122      | 0     |
| 3   | AC    | 207/239 (86%)   | 0.33   | 10 (4%) 31 19 | 30, 54, 84, 102       | 0     |
| 4   | AD    | 208/209 (99%)   | 0.14   | 5 (2%) 59 40  | 36, 57, 80, 89        | 0     |
| 5   | AE    | 151/162 (93%)   | -0.09  | 2 (1%) 77 59  | 29, 40, 59, 81        | 0     |
| 6   | AF    | 101/101 (100%)  | 0.23   | 3 (2%) 51 32  | 41, 68, 86, 99        | 0     |
| 7   | AG    | 155/156 (99%)   | 0.47   | 10 (6%) 20 11 | 44, 67, 112, 126      | 0     |
| 8   | AH    | 138/138 (100%)  | -0.12  | 0 100 100     | 32, 45, 63, 74        | 0     |
| 9   | AI    | 127/128 (99%)   | 0.40   | 9 (7%) 17 9   | 33, 61, 81, 90        | 0     |
| 10  | AJ    | 99/105 (94%)    | 0.50   | 9 (9%) 10 5   | 38, 58, 100, 104      | 0     |
| 11  | AK    | 119/129 (92%)   | 0.27   | 4 (3%) 46 29  | 26, 53, 76, 94        | 0     |
| 12  | AL    | 125/132 (94%)   | 0.27   | 7 (5%) 25 14  | 27, 45, 64, 96        | 0     |
| 13  | AM    | 119/126 (94%)   | 1.02   | 19 (15%) 2 1  | 46, 83, 107, 117      | 0     |
| 14  | AN    | 60/61 (98%)     | 0.40   | 7 (11%) 5 3   | 35, 48, 83, 91        | 0     |
| 15  | AO    | 88/89 (98%)     | 0.19   | 2 (2%) 61 41  | 33, 51, 75, 85        | 0     |
| 16  | AP    | 84/88 (95%)     | 0.15   | 1 (1%) 79 61  | 37, 47, 70, 95        | 0     |
| 17  | AQ    | 100/105 (95%)   | -0.08  | 0 100 100     | 27, 44, 62, 65        | 0     |
| 18  | AR    | 70/88 (79%)     | 0.26   | 2 (2%) 52 33  | 36, 57, 94, 95        | 0     |
| 19  | AS    | 88/93 (94%)     | 0.83   | 8 (9%) 10 5   | 59, 82, 103, 109      | 0     |
| 20  | AT    | 99/106 (93%)    | 0.12   | 3 (3%) 51 32  | 33, 45, 68, 73        | 0     |
| 21  | AU    | 25/27 (92%)     | 1.01   | 2 (8%) 13 7   | 43, 59, 79, 81        | 0     |
| 22  | AV    | 76/76 (100%)    | 0.41   | 5 (6%) 19 11  | 33, 74, 111, 145      | 0     |
| 23  | AX    | 9/9 (100%)      | 1.19   | 3 (33%) 0 0   | 28, 51, 122, 134      | 0     |
| 24  | AY    | 687/691 (99%)   | 0.53   | 62 (9%) 10 6  | 39, 67, 119, 141      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25  | B0    | 84/84 (100%)    | 1.78   | 15 (17%) 2 1   | 43, 56, 121, 140      | 0     |
| 26  | B1    | 94/97 (96%)     | 0.48   | 6 (6%) 20 11   | 26, 47, 76, 88        | 0     |
| 27  | B2    | 71/71 (100%)    | 0.62   | 7 (9%) 8 5     | 41, 57, 88, 112       | 0     |
| 28  | B3    | 60/60 (100%)    | 0.58   | 2 (3%) 47 30   | 35, 56, 75, 100       | 0     |
| 29  | B4    | 71/71 (100%)    | 3.83   | 61 (85%) 0 0   | 129, 151, 159, 159    | 0     |
| 30  | B5    | 59/59 (100%)    | 0.60   | 7 (11%) 5 2    | 20, 42, 109, 122      | 0     |
| 31  | B6    | 50/53 (94%)     | 1.51   | 11 (22%) 1 1   | 41, 72, 91, 98        | 0     |
| 32  | B7    | 48/48 (100%)    | 0.00   | 1 (2%) 64 45   | 18, 30, 60, 86        | 0     |
| 33  | B8    | 64/64 (100%)    | 0.63   | 8 (12%) 4 2    | 32, 49, 70, 87        | 0     |
| 34  | B9    | 37/37 (100%)    | 0.66   | 2 (5%) 26 16   | 40, 52, 62, 76        | 0     |
| 35  | BA    | 2901/2915 (99%) | 0.19   | 107 (3%) 42 27 | 18, 42, 116, 244      | 0     |
| 36  | BB    | 119/122 (97%)   | 0.20   | 1 (0%) 86 71   | 42, 88, 115, 130      | 0     |
| 37  | BC    | 227/228 (99%)   | 0.82   | 35 (15%) 2 1   | 25, 78, 124, 135      | 0     |
| 38  | BD    | 275/275 (100%)  | -0.00  | 8 (2%) 52 33   | 18, 32, 58, 93        | 0     |
| 39  | BE    | 205/206 (99%)   | 0.34   | 12 (5%) 23 14  | 23, 42, 78, 86        | 0     |
| 40  | BF    | 208/210 (99%)   | 0.42   | 16 (7%) 14 8   | 17, 52, 104, 121      | 0     |
| 41  | BG    | 179/181 (98%)   | 1.47   | 51 (28%) 1 0   | 94, 122, 138, 144     | 0     |
| 42  | BH    | 176/180 (97%)   | 0.90   | 21 (11%) 5 2   | 52, 75, 97, 108       | 0     |
| 43  | BJ    | 1/130 (0%)      | 2.80   | 1 (100%) 0 0   | 121, 121, 121, 121    | 0     |
| 44  | BK    | 0/140           | -      | -              | -                     | -     |
| 45  | BL    | 0/71            | -      | -              | -                     | -     |
| 46  | BN    | 139/140 (99%)   | 0.13   | 5 (3%) 43 27   | 31, 45, 72, 93        | 0     |
| 47  | BO    | 122/122 (100%)  | -0.26  | 0 100 100      | 25, 39, 54, 63        | 0     |
| 48  | BP    | 146/149 (97%)   | 1.24   | 28 (19%) 1 1   | 34, 67, 96, 118       | 0     |
| 49  | BQ    | 141/141 (100%)  | 0.21   | 3 (2%) 64 45   | 33, 49, 75, 115       | 0     |
| 50  | BR    | 117/117 (100%)  | 0.12   | 4 (3%) 46 29   | 23, 40, 59, 67        | 0     |
| 51  | BS    | 99/111 (89%)    | 1.00   | 14 (14%) 3 1   | 68, 91, 113, 122      | 0     |
| 52  | BT    | 138/146 (94%)   | 0.95   | 23 (16%) 2 1   | 32, 53, 122, 144      | 0     |
| 53  | BU    | 117/117 (100%)  | -0.05  | 2 (1%) 70 51   | 28, 42, 69, 85        | 0     |
| 54  | BV    | 101/101 (100%)  | 0.41   | 7 (6%) 18 10   | 25, 62, 83, 87        | 0     |
| 55  | BW    | 113/113 (100%)  | 0.14   | 5 (4%) 35 21   | 26, 38, 69, 104       | 0     |
| 56  | BX    | 93/95 (97%)     | -0.15  | 2 (2%) 62 43   | 30, 41, 58, 63        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 57  | BY    | 101/109 (92%)     | 1.29   | 23 (22%) 1 1   | 37, 61, 118, 127      | 0     |
| 58  | BZ    | 185/205 (90%)     | 0.85   | 27 (14%) 3 1   | 25, 81, 96, 109       | 0     |
| All | All   | 11218/11801 (95%) | 0.38   | 759 (6%) 18 10 | 17, 52, 116, 244      | 0     |

All (759) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 35  | BA    | 654(E) | G    | 16.7 |
| 24  | AY    | 48     | GLY  | 16.4 |
| 39  | BE    | 205    | ALA  | 15.5 |
| 25  | B0    | 3      | HIS  | 15.2 |
| 49  | BQ    | 141    | GLN  | 13.7 |
| 13  | AM    | 120    | LYS  | 13.6 |
| 35  | BA    | 654(V) | A    | 13.5 |
| 25  | B0    | 7      | LEU  | 13.1 |
| 49  | BQ    | 140    | ALA  | 13.0 |
| 57  | BY    | 51     | VAL  | 12.9 |
| 35  | BA    | 1534   | U    | 12.8 |
| 24  | AY    | 50     | ALA  | 12.2 |
| 35  | BA    | 654(I) | C    | 12.0 |
| 35  | BA    | 654(H) | G    | 11.1 |
| 24  | AY    | 573    | HIS  | 11.0 |
| 35  | BA    | 654(G) | C    | 11.0 |
| 25  | B0    | 5      | LYS  | 10.9 |
| 35  | BA    | 2802   | G    | 10.9 |
| 25  | B0    | 4      | LYS  | 10.9 |
| 25  | B0    | 2      | ALA  | 10.8 |
| 11  | AK    | 129    | SER  | 10.5 |
| 24  | AY    | 690    | GLY  | 9.9  |
| 35  | BA    | 2796   | U    | 9.8  |
| 24  | AY    | 46     | HIS  | 9.6  |
| 11  | AK    | 128    | ALA  | 9.6  |
| 35  | BA    | 654(F) | C    | 9.4  |
| 25  | B0    | 6      | GLY  | 9.2  |
| 35  | BA    | 654(K) | C    | 8.9  |
| 19  | AS    | 91     | LYS  | 8.8  |
| 24  | AY    | 52     | MET  | 8.8  |
| 35  | BA    | 1077   | A    | 8.7  |
| 35  | BA    | 654(L) | G    | 8.6  |
| 24  | AY    | 51     | THR  | 8.4  |
| 35  | BA    | 2795   | G    | 8.3  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 12  | AL    | 129    | ALA  | 8.2  |
| 13  | AM    | 119    | GLY  | 8.2  |
| 30  | B5    | 2      | ALA  | 8.1  |
| 1   | AA    | 83     | U    | 8.0  |
| 29  | B4    | 63     | TYR  | 7.8  |
| 35  | BA    | 654(D) | G    | 7.7  |
| 24  | AY    | 5      | VAL  | 7.7  |
| 29  | B4    | 71     | ARG  | 7.7  |
| 57  | BY    | 52     | SER  | 7.7  |
| 35  | BA    | 2793   | G    | 7.7  |
| 35  | BA    | 2803   | C    | 7.6  |
| 25  | B0    | 8      | GLY  | 7.6  |
| 34  | B9    | 1      | MET  | 7.5  |
| 38  | BD    | 276    | LYS  | 7.5  |
| 48  | BP    | 149    | GLU  | 7.5  |
| 35  | BA    | 2799   | C    | 7.4  |
| 29  | B4    | 67     | TYR  | 7.4  |
| 29  | B4    | 25     | TYR  | 7.4  |
| 40  | BF    | 12     | LEU  | 7.3  |
| 37  | BC    | 105    | LEU  | 7.3  |
| 29  | B4    | 64     | GLY  | 7.2  |
| 31  | B6    | 31     | PRO  | 7.1  |
| 35  | BA    | 2805   | G    | 7.1  |
| 24  | AY    | 537    | GLU  | 7.1  |
| 35  | BA    | 654(C) | G    | 7.1  |
| 40  | BF    | 11     | VAL  | 7.1  |
| 39  | BE    | 204    | ALA  | 7.0  |
| 29  | B4    | 47     | GLN  | 7.0  |
| 41  | BG    | 50     | ALA  | 7.0  |
| 5   | AE    | 155    | GLU  | 7.0  |
| 38  | BD    | 36     | PRO  | 6.9  |
| 21  | AU    | 26     | LYS  | 6.9  |
| 52  | BT    | 137    | LYS  | 6.8  |
| 24  | AY    | 49     | ALA  | 6.7  |
| 29  | B4    | 46     | GLN  | 6.7  |
| 29  | B4    | 68     | ARG  | 6.7  |
| 52  | BT    | 136    | GLN  | 6.7  |
| 29  | B4    | 42     | PHE  | 6.6  |
| 29  | B4    | 12     | ALA  | 6.6  |
| 30  | B5    | 58     | LEU  | 6.6  |
| 54  | BV    | 36     | PRO  | 6.6  |
| 1   | AA    | 88     | A    | 6.6  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 57  | BY    | 2       | ARG  | 6.6  |
| 35  | BA    | 2897    | U    | 6.5  |
| 35  | BA    | 275     | G    | 6.5  |
| 29  | B4    | 65      | ASP  | 6.5  |
| 13  | AM    | 84      | ILE  | 6.5  |
| 24  | AY    | 44      | GLU  | 6.5  |
| 52  | BT    | 138     | ALA  | 6.4  |
| 13  | AM    | 116     | THR  | 6.4  |
| 13  | AM    | 117     | VAL  | 6.4  |
| 35  | BA    | 2896    | C    | 6.3  |
| 40  | BF    | 1       | MET  | 6.3  |
| 40  | BF    | 10      | PRO  | 6.3  |
| 29  | B4    | 70      | GLY  | 6.3  |
| 58  | BZ    | 114     | GLY  | 6.3  |
| 35  | BA    | 2792    | G    | 6.2  |
| 42  | BH    | 176     | ALA  | 6.2  |
| 35  | BA    | 2801    | A    | 6.2  |
| 52  | BT    | 1       | MET  | 6.1  |
| 37  | BC    | 126     | SER  | 6.1  |
| 29  | B4    | 62      | ARG  | 6.0  |
| 14  | AN    | 2       | ALA  | 6.0  |
| 35  | BA    | 654(U)  | A    | 5.9  |
| 35  | BA    | 2602    | A    | 5.9  |
| 24  | AY    | 503     | GLY  | 5.9  |
| 52  | BT    | 39      | ARG  | 5.9  |
| 29  | B4    | 66      | SER  | 5.8  |
| 24  | AY    | 43      | GLY  | 5.7  |
| 30  | B5    | 59      | GLU  | 5.7  |
| 35  | BA    | 1847    | A    | 5.6  |
| 1   | AA    | 1030    | C    | 5.6  |
| 1   | AA    | 89      | C    | 5.6  |
| 24  | AY    | 42      | ILE  | 5.5  |
| 22  | AV    | 17      | C    | 5.5  |
| 24  | AY    | 4       | LYS  | 5.4  |
| 52  | BT    | 32      | TYR  | 5.4  |
| 6   | AF    | 101     | ALA  | 5.4  |
| 35  | BA    | 654(J)  | A    | 5.4  |
| 35  | BA    | 2801(A) | A    | 5.4  |
| 52  | BT    | 133     | GLU  | 5.3  |
| 41  | BG    | 113     | ARG  | 5.3  |
| 35  | BA    | 654(Q)  | C    | 5.3  |
| 3   | AC    | 78      | GLY  | 5.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 29         | B4           | 39         | CYS         | 5.3         |
| 24         | AY           | 45         | VAL         | 5.3         |
| 22         | AV           | 16         | C           | 5.3         |
| 7          | AG           | 49         | ILE         | 5.2         |
| 1          | AA           | 1534       | A           | 5.2         |
| 1          | AA           | 82         | U           | 5.2         |
| 13         | AM           | 7          | VAL         | 5.2         |
| 51         | BS           | 58         | LEU         | 5.2         |
| 48         | BP           | 110        | TYR         | 5.2         |
| 40         | BF           | 24         | LEU         | 5.1         |
| 24         | AY           | 507        | TYR         | 5.1         |
| 29         | B4           | 6          | HIS         | 5.1         |
| 24         | AY           | 47         | GLU         | 5.0         |
| 3          | AC           | 130        | VAL         | 5.0         |
| 41         | BG           | 154        | GLY         | 5.0         |
| 52         | BT           | 135        | ALA         | 4.9         |
| 41         | BG           | 76         | SER         | 4.9         |
| 35         | BA           | 2894       | G           | 4.9         |
| 31         | B6           | 54         | ILE         | 4.9         |
| 35         | BA           | 2804       | C           | 4.9         |
| 35         | BA           | 1541       | G           | 4.9         |
| 29         | B4           | 61         | ARG         | 4.8         |
| 35         | BA           | 156        | U           | 4.8         |
| 35         | BA           | 2794       | C           | 4.8         |
| 35         | BA           | 654(T)     | C           | 4.8         |
| 35         | BA           | 1536       | C           | 4.8         |
| 35         | BA           | 884        | C           | 4.7         |
| 3          | AC           | 120        | VAL         | 4.7         |
| 10         | AJ           | 85         | LEU         | 4.7         |
| 40         | BF           | 7          | TYR         | 4.7         |
| 26         | B1           | 85         | LEU         | 4.7         |
| 53         | BU           | 118        | GLY         | 4.7         |
| 39         | BE           | 76         | ARG         | 4.7         |
| 1          | AA           | 1001(A)    | G           | 4.7         |
| 23         | AX           | 11         | A           | 4.7         |
| 41         | BG           | 90         | LEU         | 4.6         |
| 1          | AA           | 1493       | A           | 4.6         |
| 48         | BP           | 150        | ALA         | 4.6         |
| 1          | AA           | 1533       | C           | 4.6         |
| 37         | BC           | 96         | GLY         | 4.6         |
| 57         | BY           | 55         | TYR         | 4.6         |
| 35         | BA           | 2310       | A           | 4.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 37         | BC           | 78         | ILE         | 4.6         |
| 35         | BA           | 654        | A           | 4.5         |
| 29         | B4           | 69         | LYS         | 4.5         |
| 1          | AA           | 1031       | G           | 4.5         |
| 35         | BA           | 1535       | A           | 4.5         |
| 58         | BZ           | 179        | ASP         | 4.5         |
| 24         | AY           | 538        | TYR         | 4.5         |
| 7          | AG           | 84         | ASN         | 4.5         |
| 29         | B4           | 24         | THR         | 4.5         |
| 46         | BN           | 3          | THR         | 4.5         |
| 2          | AB           | 7          | VAL         | 4.5         |
| 35         | BA           | 1174       | A           | 4.5         |
| 29         | B4           | 48         | ARG         | 4.5         |
| 1          | AA           | 1032       | G           | 4.5         |
| 2          | AB           | 16         | HIS         | 4.5         |
| 42         | BH           | 2          | SER         | 4.4         |
| 27         | B2           | 71         | ASN         | 4.4         |
| 42         | BH           | 83         | TYR         | 4.4         |
| 52         | BT           | 28         | VAL         | 4.4         |
| 41         | BG           | 4          | ASP         | 4.4         |
| 41         | BG           | 51         | ARG         | 4.4         |
| 28         | B3           | 1          | MET         | 4.4         |
| 42         | BH           | 168        | PRO         | 4.4         |
| 24         | AY           | 539        | ILE         | 4.3         |
| 41         | BG           | 128        | ARG         | 4.3         |
| 29         | B4           | 1          | MET         | 4.3         |
| 35         | BA           | 654(S)     | G           | 4.3         |
| 29         | B4           | 7          | PRO         | 4.3         |
| 40         | BF           | 208        | GLY         | 4.3         |
| 24         | AY           | 500        | GLN         | 4.3         |
| 1          | AA           | 1030(B)    | C           | 4.3         |
| 1          | AA           | 1129       | C           | 4.3         |
| 41         | BG           | 118        | ARG         | 4.2         |
| 54         | BV           | 48         | GLY         | 4.2         |
| 41         | BG           | 41         | GLN         | 4.2         |
| 33         | B8           | 48         | PHE         | 4.2         |
| 52         | BT           | 30         | VAL         | 4.2         |
| 12         | AL           | 28         | LYS         | 4.2         |
| 29         | B4           | 28         | LYS         | 4.2         |
| 24         | AY           | 536        | LYS         | 4.2         |
| 1          | AA           | 1030(A)    | G           | 4.1         |
| 13         | AM           | 118        | ALA         | 4.1         |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 41  | BG    | 102     | PHE  | 4.1  |
| 37  | BC    | 114     | VAL  | 4.1  |
| 57  | BY    | 58      | GLY  | 4.1  |
| 52  | BT    | 27      | THR  | 4.1  |
| 53  | BU    | 91      | ASP  | 4.1  |
| 29  | B4    | 58      | ARG  | 4.1  |
| 35  | BA    | 352     | G    | 4.1  |
| 35  | BA    | 654(N)  | G    | 4.1  |
| 35  | BA    | 2892    | A    | 4.1  |
| 57  | BY    | 89      | PHE  | 4.1  |
| 55  | BW    | 112     | GLY  | 4.1  |
| 14  | AN    | 14      | PRO  | 4.0  |
| 29  | B4    | 37      | SER  | 4.1  |
| 37  | BC    | 106     | ASP  | 4.0  |
| 29  | B4    | 5       | ILE  | 4.0  |
| 30  | B5    | 55      | ARG  | 4.0  |
| 1   | AA    | 1036    | G    | 4.0  |
| 29  | B4    | 27      | THR  | 4.0  |
| 1   | AA    | 1026    | G    | 4.0  |
| 51  | BS    | 54      | LEU  | 4.0  |
| 35  | BA    | 1066    | U    | 4.0  |
| 24  | AY    | 6       | GLU  | 4.0  |
| 38  | BD    | 275     | LYS  | 3.9  |
| 57  | BY    | 54      | LYS  | 3.9  |
| 39  | BE    | 132     | HIS  | 3.9  |
| 35  | BA    | 1076    | C    | 3.9  |
| 1   | AA    | 1030(D) | A    | 3.9  |
| 24  | AY    | 571     | SER  | 3.9  |
| 29  | B4    | 10      | VAL  | 3.9  |
| 32  | B7    | 48      | LYS  | 3.9  |
| 58  | BZ    | 150     | LEU  | 3.9  |
| 20  | AT    | 100     | ILE  | 3.8  |
| 39  | BE    | 72      | VAL  | 3.8  |
| 57  | BY    | 56      | PRO  | 3.8  |
| 20  | AT    | 9       | ASN  | 3.8  |
| 24  | AY    | 504     | ARG  | 3.8  |
| 13  | AM    | 85      | GLY  | 3.8  |
| 57  | BY    | 53      | PRO  | 3.8  |
| 29  | B4    | 40      | HIS  | 3.8  |
| 29  | B4    | 52      | THR  | 3.8  |
| 41  | BG    | 82      | LEU  | 3.8  |
| 42  | BH    | 42      | ARG  | 3.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 29         | B4           | 22         | ILE         | 3.8         |
| 35         | BA           | 1173       | G           | 3.8         |
| 48         | BP           | 51         | PHE         | 3.8         |
| 3          | AC           | 127        | ARG         | 3.7         |
| 9          | AI           | 61         | ALA         | 3.7         |
| 12         | AL           | 128        | ALA         | 3.7         |
| 24         | AY           | 501        | THR         | 3.7         |
| 3          | AC           | 169        | ALA         | 3.7         |
| 24         | AY           | 540        | PRO         | 3.7         |
| 58         | BZ           | 187        | ALA         | 3.7         |
| 35         | BA           | 887        | A           | 3.7         |
| 29         | B4           | 31         | ILE         | 3.7         |
| 41         | BG           | 26         | GLN         | 3.7         |
| 37         | BC           | 122        | GLY         | 3.7         |
| 31         | B6           | 42         | TRP         | 3.7         |
| 35         | BA           | 881        | G           | 3.7         |
| 51         | BS           | 57         | LYS         | 3.7         |
| 24         | AY           | 534        | ILE         | 3.7         |
| 29         | B4           | 19         | GLY         | 3.7         |
| 31         | B6           | 46         | HIS         | 3.7         |
| 58         | BZ           | 176        | PRO         | 3.7         |
| 29         | B4           | 13         | ARG         | 3.6         |
| 57         | BY           | 61         | ILE         | 3.6         |
| 42         | BH           | 85         | LYS         | 3.6         |
| 35         | BA           | 2807       | G           | 3.6         |
| 7          | AG           | 79         | ARG         | 3.6         |
| 19         | AS           | 90         | THR         | 3.6         |
| 35         | BA           | 1176       | G           | 3.6         |
| 35         | BA           | 508        | G           | 3.6         |
| 22         | AV           | 20         | U           | 3.6         |
| 4          | AD           | 209        | ARG         | 3.6         |
| 24         | AY           | 508        | GLY         | 3.6         |
| 24         | AY           | 531        | GLY         | 3.6         |
| 57         | BY           | 3          | VAL         | 3.6         |
| 58         | BZ           | 115        | GLY         | 3.6         |
| 35         | BA           | 277        | C           | 3.6         |
| 35         | BA           | 1509       | C           | 3.6         |
| 39         | BE           | 88         | GLY         | 3.6         |
| 29         | B4           | 21         | VAL         | 3.6         |
| 2          | AB           | 19         | HIS         | 3.6         |
| 55         | BW           | 111        | HIS         | 3.6         |
| 29         | B4           | 43         | TYR         | 3.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 37         | BC           | 86         | GLU         | 3.5         |
| 41         | BG           | 78         | SER         | 3.5         |
| 2          | AB           | 18         | GLY         | 3.5         |
| 29         | B4           | 41         | PRO         | 3.5         |
| 9          | AI           | 62         | TYR         | 3.5         |
| 41         | BG           | 148        | MET         | 3.5         |
| 29         | B4           | 15         | ILE         | 3.5         |
| 29         | B4           | 56         | VAL         | 3.5         |
| 30         | B5           | 60         | VAL         | 3.5         |
| 13         | AM           | 115        | LYS         | 3.5         |
| 35         | BA           | 654(A)     | G           | 3.5         |
| 24         | AY           | 525        | PHE         | 3.5         |
| 24         | AY           | 570        | GLY         | 3.5         |
| 48         | BP           | 50         | ARG         | 3.5         |
| 3          | AC           | 107        | GLN         | 3.5         |
| 35         | BA           | 2402       | C           | 3.5         |
| 29         | B4           | 16         | CYS         | 3.4         |
| 33         | B8           | 34         | TRP         | 3.4         |
| 57         | BY           | 50         | ARG         | 3.4         |
| 29         | B4           | 36         | CYS         | 3.4         |
| 41         | BG           | 25         | TYR         | 3.4         |
| 35         | BA           | 883        | G           | 3.4         |
| 58         | BZ           | 184        | ALA         | 3.4         |
| 1          | AA           | 1025       | U           | 3.4         |
| 21         | AU           | 25         | LYS         | 3.4         |
| 7          | AG           | 156        | TRP         | 3.4         |
| 48         | BP           | 118        | GLY         | 3.4         |
| 27         | B2           | 68         | ARG         | 3.4         |
| 57         | BY           | 60         | PHE         | 3.4         |
| 51         | BS           | 107        | GLU         | 3.4         |
| 38         | BD           | 244        | ARG         | 3.4         |
| 10         | AJ           | 55         | LYS         | 3.3         |
| 41         | BG           | 45         | GLU         | 3.3         |
| 3          | AC           | 119        | ARG         | 3.3         |
| 12         | AL           | 127        | GLU         | 3.3         |
| 26         | B1           | 57         | GLU         | 3.3         |
| 37         | BC           | 72         | GLN         | 3.3         |
| 51         | BS           | 82         | ILE         | 3.3         |
| 2          | AB           | 15         | VAL         | 3.3         |
| 27         | B2           | 16         | LEU         | 3.3         |
| 48         | BP           | 53         | GLY         | 3.3         |
| 35         | BA           | 2207       | G           | 3.3         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 58         | BZ           | 186        | GLU         | 3.3         |
| 37         | BC           | 206        | LYS         | 3.3         |
| 58         | BZ           | 148        | ASP         | 3.3         |
| 35         | BA           | 276        | A           | 3.3         |
| 37         | BC           | 128        | LEU         | 3.3         |
| 48         | BP           | 27         | HIS         | 3.3         |
| 1          | AA           | 1257       | U           | 3.2         |
| 51         | BS           | 68         | GLN         | 3.2         |
| 9          | AI           | 126        | SER         | 3.2         |
| 29         | B4           | 11         | PRO         | 3.2         |
| 2          | AB           | 122        | PHE         | 3.2         |
| 27         | B2           | 72         | ALA         | 3.2         |
| 58         | BZ           | 166        | SER         | 3.2         |
| 29         | B4           | 23         | GLU         | 3.2         |
| 35         | BA           | 229        | A           | 3.2         |
| 35         | BA           | 654(M)     | C           | 3.2         |
| 24         | AY           | 582        | PHE         | 3.2         |
| 39         | BE           | 54         | GLN         | 3.2         |
| 37         | BC           | 123        | ALA         | 3.2         |
| 24         | AY           | 502        | GLY         | 3.2         |
| 57         | BY           | 57         | GLN         | 3.2         |
| 5          | AE           | 154        | GLY         | 3.1         |
| 13         | AM           | 10         | PRO         | 3.1         |
| 41         | BG           | 126        | ASP         | 3.1         |
| 35         | BA           | 888        | C           | 3.1         |
| 24         | AY           | 530        | VAL         | 3.1         |
| 25         | B0           | 76         | GLY         | 3.1         |
| 42         | BH           | 155        | SER         | 3.1         |
| 9          | AI           | 4          | TYR         | 3.1         |
| 40         | BF           | 13         | SER         | 3.1         |
| 40         | BF           | 25         | PRO         | 3.1         |
| 48         | BP           | 91         | PHE         | 3.1         |
| 27         | B2           | 45         | SER         | 3.1         |
| 54         | BV           | 30         | GLY         | 3.1         |
| 52         | BT           | 134        | GLU         | 3.1         |
| 29         | B4           | 49         | PHE         | 3.1         |
| 29         | B4           | 59         | PHE         | 3.1         |
| 13         | AM           | 4          | ILE         | 3.1         |
| 52         | BT           | 91         | ARG         | 3.1         |
| 52         | BT           | 34         | VAL         | 3.1         |
| 35         | BA           | 885        | C           | 3.1         |
| 48         | BP           | 15         | ARG         | 3.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | AS    | 41   | VAL  | 3.0  |
| 37  | BC    | 124  | VAL  | 3.0  |
| 41  | BG    | 117  | PHE  | 3.0  |
| 19  | AS    | 30   | LEU  | 3.0  |
| 48  | BP    | 52   | GLU  | 3.0  |
| 58  | BZ    | 168  | GLU  | 3.0  |
| 33  | B8    | 64   | TYR  | 3.0  |
| 3   | AC    | 168  | ALA  | 3.0  |
| 2   | AB    | 128  | GLU  | 3.0  |
| 35  | BA    | 896  | A    | 3.0  |
| 35  | BA    | 1848 | A    | 3.0  |
| 29  | B4    | 57   | GLU  | 3.0  |
| 57  | BY    | 91   | GLU  | 3.0  |
| 19  | AS    | 89   | ALA  | 3.0  |
| 37  | BC    | 113  | ALA  | 3.0  |
| 1   | AA    | 84   | U    | 3.0  |
| 23  | AX    | 19   | A    | 3.0  |
| 24  | AY    | 203  | GLU  | 3.0  |
| 1   | AA    | 204  | U    | 3.0  |
| 1   | AA    | 841  | U    | 3.0  |
| 24  | AY    | 583  | LYS  | 3.0  |
| 7   | AG    | 72   | ARG  | 3.0  |
| 35  | BA    | 886  | C    | 3.0  |
| 2   | AB    | 140  | HIS  | 3.0  |
| 7   | AG    | 151  | TYR  | 2.9  |
| 52  | BT    | 115  | ARG  | 2.9  |
| 57  | BY    | 87   | LYS  | 2.9  |
| 10  | AJ    | 4    | ILE  | 2.9  |
| 24  | AY    | 574  | GLU  | 2.9  |
| 40  | BF    | 23   | ASP  | 2.9  |
| 42  | BH    | 81   | GLU  | 2.9  |
| 12  | AL    | 19   | ARG  | 2.9  |
| 24  | AY    | 509  | HIS  | 2.9  |
| 41  | BG    | 43   | LEU  | 2.9  |
| 3   | AC    | 81   | GLY  | 2.9  |
| 2   | AB    | 230  | VAL  | 2.9  |
| 48  | BP    | 48   | PRO  | 2.9  |
| 35  | BA    | 2140 | C    | 2.9  |
| 52  | BT    | 106  | SER  | 2.9  |
| 37  | BC    | 121  | MET  | 2.9  |
| 1   | AA    | 1002 | G    | 2.9  |
| 52  | BT    | 112  | ARG  | 2.9  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | B0           | 74         | ARG         | 2.9         |
| 37         | BC           | 53         | ARG         | 2.9         |
| 24         | AY           | 569        | ASP         | 2.9         |
| 37         | BC           | 81         | GLY         | 2.9         |
| 48         | BP           | 23         | PRO         | 2.9         |
| 24         | AY           | 197        | ARG         | 2.9         |
| 58         | BZ           | 63         | ASP         | 2.9         |
| 57         | BY           | 28         | LYS         | 2.9         |
| 35         | BA           | 271(L)     | U           | 2.9         |
| 40         | BF           | 14         | PRO         | 2.9         |
| 41         | BG           | 178        | PHE         | 2.9         |
| 24         | AY           | 578        | SER         | 2.9         |
| 11         | AK           | 11         | LYS         | 2.9         |
| 19         | AS           | 85         | LYS         | 2.9         |
| 29         | B4           | 45         | GLY         | 2.9         |
| 29         | B4           | 44         | THR         | 2.8         |
| 25         | B0           | 79         | VAL         | 2.8         |
| 35         | BA           | 1068       | G           | 2.8         |
| 29         | B4           | 30         | GLU         | 2.8         |
| 10         | AJ           | 89         | ASP         | 2.8         |
| 11         | AK           | 127        | LYS         | 2.8         |
| 57         | BY           | 4          | LYS         | 2.8         |
| 1          | AA           | 78         | G           | 2.8         |
| 42         | BH           | 9          | ILE         | 2.8         |
| 13         | AM           | 8          | GLU         | 2.8         |
| 29         | B4           | 8          | LYS         | 2.8         |
| 29         | B4           | 50         | VAL         | 2.8         |
| 43         | BJ           | 85         | LEU         | 2.8         |
| 42         | BH           | 47         | GLU         | 2.8         |
| 58         | BZ           | 33         | LEU         | 2.8         |
| 40         | BF           | 17         | ARG         | 2.8         |
| 51         | BS           | 43         | GLU         | 2.8         |
| 42         | BH           | 1          | MET         | 2.8         |
| 58         | BZ           | 177        | PRO         | 2.8         |
| 41         | BG           | 165        | THR         | 2.8         |
| 31         | B6           | 9          | LEU         | 2.8         |
| 33         | B8           | 65         | GLU         | 2.8         |
| 7          | AG           | 83         | ALA         | 2.8         |
| 42         | BH           | 172        | LYS         | 2.8         |
| 55         | BW           | 113        | LYS         | 2.8         |
| 41         | BG           | 94         | LEU         | 2.7         |
| 46         | BN           | 1          | MET         | 2.7         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 29         | B4           | 17         | GLY         | 2.7         |
| 1          | AA           | 81         | U           | 2.7         |
| 24         | AY           | 563        | ILE         | 2.7         |
| 41         | BG           | 125        | PHE         | 2.7         |
| 58         | BZ           | 13         | GLU         | 2.7         |
| 31         | B6           | 37         | ARG         | 2.7         |
| 52         | BT           | 29         | ARG         | 2.7         |
| 52         | BT           | 33         | LYS         | 2.7         |
| 10         | AJ           | 83         | GLU         | 2.7         |
| 35         | BA           | 654(O)     | G           | 2.7         |
| 35         | BA           | 2139       | C           | 2.7         |
| 48         | BP           | 95         | VAL         | 2.7         |
| 2          | AB           | 137        | ARG         | 2.7         |
| 14         | AN           | 15         | LYS         | 2.7         |
| 57         | BY           | 81         | LYS         | 2.7         |
| 35         | BA           | 1026       | U           | 2.7         |
| 50         | BR           | 8          | ARG         | 2.7         |
| 1          | AA           | 90         | U           | 2.7         |
| 31         | B6           | 7          | ILE         | 2.7         |
| 58         | BZ           | 68         | PRO         | 2.7         |
| 58         | BZ           | 161        | VAL         | 2.7         |
| 41         | BG           | 48         | GLU         | 2.7         |
| 37         | BC           | 115        | VAL         | 2.7         |
| 37         | BC           | 143        | ALA         | 2.7         |
| 9          | AI           | 60         | ASP         | 2.6         |
| 42         | BH           | 171        | LEU         | 2.6         |
| 19         | AS           | 86         | GLU         | 2.6         |
| 39         | BE           | 154        | LYS         | 2.6         |
| 46         | BN           | 68         | GLU         | 2.6         |
| 2          | AB           | 37         | ASN         | 2.6         |
| 35         | BA           | 654(R)     | C           | 2.6         |
| 24         | AY           | 689        | LYS         | 2.6         |
| 41         | BG           | 104        | GLU         | 2.6         |
| 52         | BT           | 31         | SER         | 2.6         |
| 50         | BR           | 105        | ARG         | 2.6         |
| 37         | BC           | 80         | LYS         | 2.6         |
| 41         | BG           | 180        | PHE         | 2.6         |
| 28         | B3           | 55         | ARG         | 2.6         |
| 30         | B5           | 57         | VAL         | 2.6         |
| 37         | BC           | 177        | GLY         | 2.6         |
| 37         | BC           | 168        | LYS         | 2.6         |
| 35         | BA           | 1078       | U           | 2.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 37         | BC           | 76         | LEU         | 2.6         |
| 48         | BP           | 107        | LYS         | 2.6         |
| 16         | AP           | 83         | GLU         | 2.6         |
| 1          | AA           | 1033       | G           | 2.6         |
| 33         | B8           | 35         | GLN         | 2.6         |
| 24         | AY           | 526        | VAL         | 2.6         |
| 13         | AM           | 5          | ALA         | 2.6         |
| 31         | B6           | 29         | ASN         | 2.6         |
| 41         | BG           | 75         | LYS         | 2.6         |
| 1          | AA           | 1399       | C           | 2.6         |
| 37         | BC           | 109        | MET         | 2.6         |
| 30         | B5           | 51         | TYR         | 2.6         |
| 4          | AD           | 151        | LYS         | 2.6         |
| 10         | AJ           | 100        | THR         | 2.6         |
| 41         | BG           | 145        | THR         | 2.6         |
| 35         | BA           | 272(A)     | U           | 2.6         |
| 12         | AL           | 47         | LYS         | 2.6         |
| 18         | AR           | 46         | GLU         | 2.5         |
| 24         | AY           | 232        | LEU         | 2.5         |
| 26         | B1           | 28         | GLY         | 2.5         |
| 29         | B4           | 18         | CYS         | 2.5         |
| 27         | B2           | 10         | LEU         | 2.5         |
| 35         | BA           | 2808       | U           | 2.5         |
| 42         | BH           | 167        | GLU         | 2.5         |
| 50         | BR           | 3          | HIS         | 2.5         |
| 31         | B6           | 39         | TYR         | 2.5         |
| 58         | BZ           | 162        | GLU         | 2.5         |
| 41         | BG           | 182        | LYS         | 2.5         |
| 48         | BP           | 47         | ASP         | 2.5         |
| 35         | BA           | 34         | C           | 2.5         |
| 35         | BA           | 654(B)     | C           | 2.5         |
| 41         | BG           | 73         | ALA         | 2.5         |
| 25         | B0           | 12         | ASN         | 2.5         |
| 41         | BG           | 77         | ILE         | 2.5         |
| 41         | BG           | 136        | ARG         | 2.5         |
| 41         | BG           | 139        | LEU         | 2.5         |
| 42         | BH           | 88         | LEU         | 2.5         |
| 48         | BP           | 147        | LEU         | 2.5         |
| 1          | AA           | 162        | A           | 2.5         |
| 35         | BA           | 614(B)     | G           | 2.5         |
| 42         | BH           | 23         | ARG         | 2.5         |
| 51         | BS           | 60         | GLY         | 2.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 58         | BZ           | 146        | ILE         | 2.5         |
| 22         | AV           | 47         | U           | 2.5         |
| 35         | BA           | 545        | C           | 2.5         |
| 15         | AO           | 89         | GLY         | 2.5         |
| 40         | BF           | 18         | ARG         | 2.5         |
| 54         | BV           | 101        | GLY         | 2.5         |
| 41         | BG           | 173        | LEU         | 2.5         |
| 41         | BG           | 49         | ASP         | 2.5         |
| 2          | AB           | 126        | GLU         | 2.5         |
| 14         | AN           | 19         | ARG         | 2.5         |
| 24         | AY           | 581        | ALA         | 2.5         |
| 29         | B4           | 32         | TYR         | 2.5         |
| 37         | BC           | 170        | GLY         | 2.5         |
| 40         | BF           | 207        | GLY         | 2.5         |
| 24         | AY           | 529        | ILE         | 2.5         |
| 57         | BY           | 44         | ILE         | 2.5         |
| 14         | AN           | 16         | PHE         | 2.5         |
| 35         | BA           | 2893       | G           | 2.5         |
| 1          | AA           | 470        | C           | 2.5         |
| 1          | AA           | 1532       | U           | 2.5         |
| 37         | BC           | 98         | GLU         | 2.4         |
| 48         | BP           | 94         | GLU         | 2.4         |
| 25         | B0           | 65         | GLY         | 2.4         |
| 29         | B4           | 53         | GLU         | 2.4         |
| 41         | BG           | 155        | MET         | 2.4         |
| 1          | AA           | 702        | A           | 2.4         |
| 35         | BA           | 1301       | A           | 2.4         |
| 58         | BZ           | 185        | GLU         | 2.4         |
| 7          | AG           | 48         | LYS         | 2.4         |
| 1          | AA           | 92         | C           | 2.4         |
| 41         | BG           | 150        | ASP         | 2.4         |
| 35         | BA           | 1046       | A           | 2.4         |
| 41         | BG           | 34         | LEU         | 2.4         |
| 48         | BP           | 139        | LYS         | 2.4         |
| 24         | AY           | 576        | ASP         | 2.4         |
| 39         | BE           | 61         | ARG         | 2.4         |
| 37         | BC           | 142        | LYS         | 2.4         |
| 1          | AA           | 1037       | C           | 2.4         |
| 41         | BG           | 103        | LEU         | 2.4         |
| 35         | BA           | 890        | A           | 2.4         |
| 42         | BH           | 170        | ARG         | 2.4         |
| 52         | BT           | 118        | ARG         | 2.4         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 41         | BG           | 156        | ASP         | 2.4         |
| 6          | AF           | 100        | ASN         | 2.4         |
| 29         | B4           | 26         | SER         | 2.4         |
| 33         | B8           | 33         | ASN         | 2.4         |
| 35         | BA           | 2610       | C           | 2.4         |
| 58         | BZ           | 144        | LEU         | 2.4         |
| 52         | BT           | 129        | ARG         | 2.4         |
| 55         | BW           | 63         | ASP         | 2.4         |
| 14         | AN           | 17         | LYS         | 2.4         |
| 41         | BG           | 83         | ARG         | 2.4         |
| 37         | BC           | 151        | GLY         | 2.3         |
| 42         | BH           | 116        | GLU         | 2.3         |
| 2          | AB           | 237        | ALA         | 2.3         |
| 35         | BA           | 899        | A           | 2.3         |
| 35         | BA           | 2790       | A           | 2.3         |
| 9          | AI           | 25         | LYS         | 2.3         |
| 35         | BA           | 614(A)     | U           | 2.3         |
| 38         | BD           | 262        | ARG         | 2.3         |
| 31         | B6           | 23         | THR         | 2.3         |
| 1          | AA           | 1034       | G           | 2.3         |
| 1          | AA           | 1504       | G           | 2.3         |
| 26         | B1           | 27         | GLU         | 2.3         |
| 41         | BG           | 39         | ILE         | 2.3         |
| 7          | AG           | 155        | ARG         | 2.3         |
| 35         | BA           | 155        | U           | 2.3         |
| 29         | B4           | 54         | GLY         | 2.3         |
| 54         | BV           | 19         | LYS         | 2.3         |
| 6          | AF           | 47         | ARG         | 2.3         |
| 13         | AM           | 15         | VAL         | 2.3         |
| 2          | AB           | 125        | PRO         | 2.3         |
| 24         | AY           | 53         | ASP         | 2.3         |
| 37         | BC           | 79         | ALA         | 2.3         |
| 19         | AS           | 32         | LYS         | 2.3         |
| 29         | B4           | 14         | ILE         | 2.3         |
| 13         | AM           | 112        | GLY         | 2.3         |
| 49         | BQ           | 59         | ARG         | 2.3         |
| 37         | BC           | 95         | VAL         | 2.3         |
| 1          | AA           | 77         | G           | 2.3         |
| 1          | AA           | 496        | A           | 2.3         |
| 1          | AA           | 563        | A           | 2.3         |
| 58         | BZ           | 32         | HIS         | 2.3         |
| 35         | BA           | 645        | C           | 2.3         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 24         | AY           | 236        | GLU         | 2.3         |
| 24         | AY           | 23         | ALA         | 2.3         |
| 37         | BC           | 159        | ALA         | 2.3         |
| 13         | AM           | 9          | ILE         | 2.3         |
| 24         | AY           | 584        | ILE         | 2.3         |
| 24         | AY           | 497        | PHE         | 2.3         |
| 25         | B0           | 11         | ARG         | 2.3         |
| 2          | AB           | 231        | GLU         | 2.3         |
| 7          | AG           | 153        | HIS         | 2.3         |
| 48         | BP           | 122        | PRO         | 2.3         |
| 1          | AA           | 80         | G           | 2.3         |
| 56         | BX           | 66         | LEU         | 2.3         |
| 15         | AO           | 20         | GLY         | 2.3         |
| 29         | B4           | 35         | VAL         | 2.3         |
| 38         | BD           | 26         | LYS         | 2.3         |
| 48         | BP           | 121        | LYS         | 2.3         |
| 13         | AM           | 11         | ARG         | 2.3         |
| 55         | BW           | 68         | ARG         | 2.3         |
| 2          | AB           | 124        | SER         | 2.3         |
| 24         | AY           | 211        | GLU         | 2.3         |
| 24         | AY           | 580        | MET         | 2.3         |
| 41         | BG           | 157        | ILE         | 2.3         |
| 26         | B1           | 83         | GLU         | 2.3         |
| 31         | B6           | 40         | CYS         | 2.2         |
| 57         | BY           | 27         | VAL         | 2.2         |
| 48         | BP           | 65         | ARG         | 2.2         |
| 34         | B9           | 20         | HIS         | 2.2         |
| 51         | BS           | 81         | GLY         | 2.2         |
| 35         | BA           | 271(M)     | G           | 2.2         |
| 35         | BA           | 274        | G           | 2.2         |
| 2          | AB           | 132        | LYS         | 2.2         |
| 10         | AJ           | 88         | LEU         | 2.2         |
| 39         | BE           | 131        | ALA         | 2.2         |
| 48         | BP           | 24         | GLY         | 2.2         |
| 51         | BS           | 56         | LEU         | 2.2         |
| 29         | B4           | 60         | GLN         | 2.2         |
| 39         | BE           | 59         | VAL         | 2.2         |
| 42         | BH           | 97         | ARG         | 2.2         |
| 1          | AA           | 532        | A           | 2.2         |
| 1          | AA           | 1001       | A           | 2.2         |
| 1          | AA           | 1024       | G           | 2.2         |
| 33         | B8           | 32         | LEU         | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | BP    | 82   | GLY  | 2.2  |
| 57  | BY    | 79   | CYS  | 2.2  |
| 48  | BP    | 7    | ARG  | 2.2  |
| 37  | BC    | 24   | ASP  | 2.2  |
| 25  | B0    | 85   | ALA  | 2.2  |
| 12  | AL    | 41   | ARG  | 2.2  |
| 14  | AN    | 12   | ARG  | 2.2  |
| 24  | AY    | 231  | TYR  | 2.2  |
| 13  | AM    | 60   | VAL  | 2.2  |
| 24  | AY    | 565  | VAL  | 2.2  |
| 54  | BV    | 37   | VAL  | 2.2  |
| 37  | BC    | 56   | ASP  | 2.2  |
| 46  | BN    | 139  | GLU  | 2.2  |
| 35  | BA    | 1740 | G    | 2.2  |
| 48  | BP    | 71   | VAL  | 2.2  |
| 38  | BD    | 24   | ILE  | 2.2  |
| 1   | AA    | 198  | G    | 2.2  |
| 4   | AD    | 47   | ARG  | 2.2  |
| 24  | AY    | 527  | ASN  | 2.2  |
| 3   | AC    | 96   | GLY  | 2.2  |
| 1   | AA    | 97   | G    | 2.2  |
| 38  | BD    | 2    | ALA  | 2.2  |
| 27  | B2    | 48   | HIS  | 2.2  |
| 9   | AI    | 95   | LYS  | 2.2  |
| 25  | B0    | 82   | ARG  | 2.2  |
| 1   | AA    | 1499 | A    | 2.2  |
| 35  | BA    | 1045 | A    | 2.2  |
| 4   | AD    | 158  | ILE  | 2.1  |
| 35  | BA    | 158  | U    | 2.1  |
| 35  | BA    | 1420 | U    | 2.1  |
| 35  | BA    | 2611 | U    | 2.1  |
| 13  | AM    | 31   | LYS  | 2.1  |
| 35  | BA    | 2410 | G    | 2.1  |
| 36  | BB    | 67   | G    | 2.1  |
| 58  | BZ    | 11   | GLU  | 2.1  |
| 57  | BY    | 45   | VAL  | 2.1  |
| 39  | BE    | 1    | MET  | 2.1  |
| 58  | BZ    | 14   | LYS  | 2.1  |
| 37  | BC    | 118  | PRO  | 2.1  |
| 37  | BC    | 15   | VAL  | 2.1  |
| 40  | BF    | 134  | GLY  | 2.1  |
| 10  | AJ    | 87   | THR  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | AV    | 44   | G    | 2.1  |
| 35  | BA    | 1087 | G    | 2.1  |
| 2   | AB    | 131  | PRO  | 2.1  |
| 20  | AT    | 103  | GLY  | 2.1  |
| 35  | BA    | 2791 | C    | 2.1  |
| 41  | BG    | 89   | GLY  | 2.1  |
| 41  | BG    | 11   | TYR  | 2.1  |
| 1   | AA    | 1531 | A    | 2.1  |
| 29  | B4    | 20   | ASN  | 2.1  |
| 35  | BA    | 1177 | A    | 2.1  |
| 58  | BZ    | 4    | ARG  | 2.1  |
| 52  | BT    | 36   | GLU  | 2.1  |
| 35  | BA    | 157  | U    | 2.1  |
| 51  | BS    | 55   | ALA  | 2.1  |
| 41  | BG    | 79   | ASN  | 2.1  |
| 9   | AI    | 59   | PHE  | 2.1  |
| 50  | BR    | 4    | LEU  | 2.1  |
| 24  | AY    | 684  | GLN  | 2.1  |
| 35  | BA    | 11   | G    | 2.1  |
| 58  | BZ    | 80   | ARG  | 2.1  |
| 51  | BS    | 46   | VAL  | 2.1  |
| 1   | AA    | 1286 | A    | 2.1  |
| 26  | B1    | 60   | PHE  | 2.1  |
| 35  | BA    | 2403 | C    | 2.1  |
| 41  | BG    | 161  | THR  | 2.1  |
| 46  | BN    | 4    | TYR  | 2.1  |
| 4   | AD    | 49   | ARG  | 2.1  |
| 42  | BH    | 82   | GLY  | 2.1  |
| 58  | BZ    | 20   | ARG  | 2.1  |
| 18  | AR    | 23   | LYS  | 2.1  |
| 24  | AY    | 518  | PRO  | 2.1  |
| 33  | B8    | 63   | PRO  | 2.1  |
| 41  | BG    | 86   | MET  | 2.1  |
| 24  | AY    | 555  | LEU  | 2.0  |
| 9   | AI    | 88   | TYR  | 2.0  |
| 51  | BS    | 40   | ILE  | 2.0  |
| 48  | BP    | 57   | THR  | 2.0  |
| 48  | BP    | 99   | LEU  | 2.0  |
| 1   | AA    | 1042 | G    | 2.0  |
| 1   | AA    | 1335 | C    | 2.0  |
| 35  | BA    | 1075 | C    | 2.0  |
| 10  | AJ    | 90   | LEU  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | BG    | 22   | ARG  | 2.0  |
| 51  | BS    | 92   | TYR  | 2.0  |
| 2   | AB    | 149  | LEU  | 2.0  |
| 41  | BG    | 72   | ARG  | 2.0  |
| 56  | BX    | 95   | LEU  | 2.0  |
| 42  | BH    | 111  | HIS  | 2.0  |
| 40  | BF    | 21   | ALA  | 2.0  |
| 1   | AA    | 91   | C    | 2.0  |
| 1   | AA    | 1447 | A    | 2.0  |
| 23  | AX    | 12   | A    | 2.0  |
| 54  | BV    | 20   | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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   | AA    | 1615 | 1/1   | 0.88 | 0.75 | 57.87 | 51,51,51,51                | 0     |
| 59  | MG   | AA    | 1684 | 1/1   | 0.82 | 0.85 | 50.95 | 61,61,61,61                | 0     |
| 59  | MG   | BA    | 3312 | 1/1   | 0.94 | 0.52 | 47.69 | 44,44,44,44                | 0     |
| 59  | MG   | AA    | 1636 | 1/1   | 0.77 | 0.51 | 43.25 | 60,60,60,60                | 0     |
| 59  | MG   | BA    | 3174 | 1/1   | 0.54 | 0.64 | 41.92 | 97,97,97,97                | 0     |
| 59  | MG   | BA    | 3044 | 1/1   | 0.97 | 0.40 | 39.27 | 21,21,21,21                | 0     |
| 59  | MG   | BA    | 3110 | 1/1   | 0.97 | 0.49 | 30.19 | 31,31,31,31                | 0     |
| 59  | MG   | BA    | 3007 | 1/1   | 0.93 | 0.45 | 26.36 | 26,26,26,26                | 0     |
| 59  | MG   | BA    | 3071 | 1/1   | 0.94 | 0.37 | 23.13 | 22,22,22,22                | 0     |
| 59  | MG   | BA    | 3209 | 1/1   | 0.76 | 0.63 | 19.33 | 81,81,81,81                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 59  | MG   | AA    | 1623 | 1/1   | 0.98 | 0.53 | 19.05 | 33,33,33,33                 | 0     |
| 59  | MG   | AA    | 1762 | 1/1   | 0.59 | 0.41 | 18.56 | 100,100,100,100             | 0     |
| 59  | MG   | BA    | 3048 | 1/1   | 0.91 | 0.39 | 18.50 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3207 | 1/1   | 0.86 | 0.29 | 18.31 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3310 | 1/1   | 0.91 | 0.29 | 17.93 | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3006 | 1/1   | 0.97 | 0.41 | 17.44 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3094 | 1/1   | 0.98 | 0.32 | 17.34 | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3266 | 1/1   | 0.92 | 0.31 | 17.21 | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3180 | 1/1   | 0.95 | 0.34 | 17.18 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3196 | 1/1   | 0.88 | 0.38 | 17.11 | 53,53,53,53                 | 0     |
| 59  | MG   | AA    | 1649 | 1/1   | 0.93 | 0.40 | 16.59 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3077 | 1/1   | 0.94 | 0.35 | 16.55 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3024 | 1/1   | 0.88 | 0.28 | 16.43 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3149 | 1/1   | 0.96 | 0.48 | 15.93 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3277 | 1/1   | 0.94 | 0.45 | 15.87 | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3154 | 1/1   | 0.82 | 0.60 | 15.81 | 59,59,59,59                 | 0     |
| 59  | MG   | AA    | 1741 | 1/1   | 0.73 | 0.46 | 15.50 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3056 | 1/1   | 0.90 | 0.37 | 15.32 | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3120 | 1/1   | 0.95 | 0.38 | 14.92 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3172 | 1/1   | 0.96 | 0.45 | 14.49 | 31,31,31,31                 | 0     |
| 59  | MG   | AA    | 1760 | 1/1   | 0.64 | 0.67 | 14.03 | 70,70,70,70                 | 0     |
| 59  | MG   | AA    | 1604 | 1/1   | 0.85 | 0.41 | 13.90 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3279 | 1/1   | 0.59 | 0.44 | 13.82 | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3108 | 1/1   | 0.86 | 0.27 | 13.75 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3295 | 1/1   | 0.81 | 0.30 | 13.45 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3176 | 1/1   | 0.95 | 0.46 | 12.56 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3111 | 1/1   | 0.93 | 0.32 | 12.54 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3169 | 1/1   | 0.85 | 0.37 | 12.36 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3084 | 1/1   | 0.93 | 0.55 | 12.29 | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1665 | 1/1   | 0.94 | 0.42 | 12.03 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3184 | 1/1   | 0.90 | 0.24 | 11.94 | 40,40,40,40                 | 0     |
| 59  | MG   | AA    | 1733 | 1/1   | 0.93 | 0.31 | 11.90 | 67,67,67,67                 | 0     |
| 59  | MG   | AA    | 1677 | 1/1   | 0.64 | 0.37 | 11.79 | 77,77,77,77                 | 0     |
| 59  | MG   | AA    | 1616 | 1/1   | 0.94 | 0.41 | 11.11 | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1671 | 1/1   | 0.96 | 0.65 | 11.05 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3088 | 1/1   | 0.89 | 0.24 | 11.03 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3004 | 1/1   | 0.97 | 0.38 | 10.78 | 24,24,24,24                 | 0     |
| 59  | MG   | BA    | 3039 | 1/1   | 0.97 | 0.39 | 10.39 | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1645 | 1/1   | 0.92 | 0.26 | 10.31 | 22,22,22,22                 | 0     |
| 59  | MG   | B0    | 101  | 1/1   | 0.86 | 0.77 | 9.82  | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3087 | 1/1   | 0.84 | 0.34 | 9.31  | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3116 | 1/1   | 0.82 | 0.28 | 9.23 | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3109 | 1/1   | 0.98 | 0.44 | 9.05 | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3125 | 1/1   | 0.74 | 0.38 | 8.95 | 122,122,122,122             | 0     |
| 59  | MG   | BA    | 3315 | 1/1   | 0.79 | 0.35 | 8.77 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3104 | 1/1   | 0.98 | 0.32 | 8.57 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3113 | 1/1   | 0.97 | 0.52 | 8.36 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3199 | 1/1   | 0.94 | 0.27 | 8.28 | 26,26,26,26                 | 0     |
| 59  | MG   | AA    | 1756 | 1/1   | 0.84 | 0.39 | 8.27 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3153 | 1/1   | 0.85 | 0.24 | 8.12 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3139 | 1/1   | 0.93 | 0.29 | 8.08 | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1692 | 1/1   | 0.93 | 0.23 | 7.94 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3097 | 1/1   | 0.89 | 0.41 | 7.52 | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3214 | 1/1   | 0.80 | 0.31 | 7.51 | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3248 | 1/1   | 0.83 | 0.44 | 7.45 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3051 | 1/1   | 0.94 | 0.37 | 7.40 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3258 | 1/1   | 0.77 | 0.32 | 7.38 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3271 | 1/1   | 0.84 | 0.34 | 7.36 | 28,28,28,28                 | 0     |
| 59  | MG   | AA    | 1777 | 1/1   | 0.49 | 0.31 | 7.32 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3129 | 1/1   | 0.87 | 0.30 | 7.26 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3282 | 1/1   | 0.56 | 0.30 | 7.05 | 67,67,67,67                 | 0     |
| 59  | MG   | BA    | 3091 | 1/1   | 0.97 | 0.22 | 6.84 | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3053 | 1/1   | 0.91 | 0.33 | 6.77 | 24,24,24,24                 | 0     |
| 59  | MG   | AA    | 1678 | 1/1   | 0.96 | 0.35 | 6.66 | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1690 | 1/1   | 0.95 | 0.47 | 6.61 | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1724 | 1/1   | 0.74 | 0.42 | 6.40 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3313 | 1/1   | 0.96 | 0.26 | 6.33 | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3082 | 1/1   | 0.95 | 0.49 | 6.21 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3236 | 1/1   | 0.81 | 0.24 | 6.19 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3127 | 1/1   | 0.93 | 0.24 | 6.00 | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1700 | 1/1   | 0.91 | 0.32 | 5.76 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3043 | 1/1   | 0.98 | 0.23 | 5.43 | 28,28,28,28                 | 0     |
| 59  | MG   | AA    | 1639 | 1/1   | 0.66 | 0.30 | 5.26 | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3145 | 1/1   | 0.86 | 0.23 | 5.16 | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1729 | 1/1   | 0.86 | 0.47 | 4.92 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3189 | 1/1   | 0.93 | 0.19 | 4.82 | 26,26,26,26                 | 0     |
| 59  | MG   | AA    | 1625 | 1/1   | 0.96 | 0.36 | 4.80 | 17,17,17,17                 | 0     |
| 59  | MG   | BA    | 3052 | 1/1   | 0.97 | 0.31 | 4.77 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3228 | 1/1   | 0.90 | 0.32 | 4.55 | 23,23,23,23                 | 0     |
| 59  | MG   | AA    | 1686 | 1/1   | 0.90 | 0.25 | 4.52 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3210 | 1/1   | 0.95 | 0.29 | 4.50 | 23,23,23,23                 | 0     |
| 59  | MG   | AA    | 1704 | 1/1   | 0.92 | 0.37 | 4.47 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 59  | MG   | BA    | 3075 | 1/1   | 0.88 | 0.23 | 4.11  | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3257 | 1/1   | 0.94 | 0.22 | 3.73  | 43,43,43,43                 | 0     |
| 59  | MG   | AA    | 1715 | 1/1   | 0.75 | 0.24 | 3.17  | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3078 | 1/1   | 0.92 | 0.20 | 3.10  | 26,26,26,26                 | 0     |
| 60  | ZN   | AD    | 301  | 1/1   | 0.96 | 0.35 | 3.03  | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3181 | 1/1   | 0.87 | 0.18 | 2.87  | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1638 | 1/1   | 0.76 | 0.17 | 2.86  | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3298 | 1/1   | 0.93 | 0.17 | 2.80  | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3206 | 1/1   | 0.83 | 0.23 | 2.80  | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3098 | 1/1   | 0.91 | 0.23 | 2.08  | 25,25,25,25                 | 0     |
| 59  | MG   | AA    | 1653 | 1/1   | 0.94 | 0.31 | 1.97  | 19,19,19,19                 | 0     |
| 59  | MG   | AA    | 1780 | 1/1   | 0.40 | 0.18 | 1.93  | 54,54,54,54                 | 0     |
| 59  | MG   | AA    | 1682 | 1/1   | 0.96 | 0.27 | 1.81  | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3244 | 1/1   | 0.92 | 0.21 | 1.80  | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3150 | 1/1   | 0.98 | 0.16 | 1.78  | 15,15,15,15                 | 0     |
| 59  | MG   | BA    | 3232 | 1/1   | 0.89 | 0.24 | 1.77  | 33,33,33,33                 | 0     |
| 59  | MG   | AA    | 1701 | 1/1   | 0.81 | 0.17 | 1.75  | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1725 | 1/1   | 0.93 | 0.25 | 1.72  | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1673 | 1/1   | 0.94 | 0.21 | 1.41  | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1732 | 1/1   | 0.87 | 0.25 | 0.78  | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3219 | 1/1   | 0.81 | 0.16 | 0.66  | 44,44,44,44                 | 0     |
| 59  | MG   | AA    | 1719 | 1/1   | 0.93 | 0.16 | 0.58  | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3141 | 1/1   | 0.89 | 0.20 | 0.50  | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3243 | 1/1   | 0.86 | 0.23 | 0.41  | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1726 | 1/1   | 0.83 | 0.21 | 0.36  | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3289 | 1/1   | 0.89 | 0.21 | 0.33  | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1711 | 1/1   | 0.77 | 0.19 | 0.26  | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3269 | 1/1   | 0.66 | 0.16 | 0.26  | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1761 | 1/1   | 0.86 | 0.20 | 0.20  | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3171 | 1/1   | 0.97 | 0.23 | 0.17  | 19,19,19,19                 | 0     |
| 59  | MG   | BA    | 3157 | 1/1   | 0.93 | 0.17 | 0.13  | 17,17,17,17                 | 0     |
| 59  | MG   | AA    | 1722 | 1/1   | 0.82 | 0.23 | 0.13  | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1687 | 1/1   | 0.95 | 0.20 | 0.11  | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3142 | 1/1   | 0.70 | 0.20 | 0.08  | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1736 | 1/1   | 0.94 | 0.19 | -0.11 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3208 | 1/1   | 0.91 | 0.23 | -0.15 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3217 | 1/1   | 0.95 | 0.18 | -0.23 | 35,35,35,35                 | 0     |
| 61  | GCP  | AY    | 701  | 32/32 | 0.87 | 0.21 | -0.26 | 41,53,61,63                 | 0     |
| 59  | MG   | AA    | 1693 | 1/1   | 0.92 | 0.17 | -0.28 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3288 | 1/1   | 0.98 | 0.18 | -0.32 | 24,24,24,24                 | 0     |
| 59  | MG   | AA    | 1668 | 1/1   | 0.85 | 0.17 | -0.32 | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1738 | 1/1   | 0.90 | 0.17 | -0.45 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 59  | MG   | AA    | 1751 | 1/1   | 0.90 | 0.14 | -0.89 | 46,46,46,46                | 0     |
| 59  | MG   | AA    | 1749 | 1/1   | 0.88 | 0.13 | -0.89 | 38,38,38,38                | 0     |
| 59  | MG   | BA    | 3151 | 1/1   | 0.95 | 0.13 | -1.06 | 33,33,33,33                | 0     |
| 60  | ZN   | AN    | 101  | 1/1   | 1.00 | 0.13 | -1.06 | 45,45,45,45                | 0     |
| 59  | MG   | BA    | 3050 | 1/1   | 0.94 | 0.15 | -1.20 | 23,23,23,23                | 0     |
| 59  | MG   | BA    | 3319 | 1/1   | 0.96 | 0.11 | -1.47 | 35,35,35,35                | 0     |
| 59  | MG   | BA    | 3001 | 1/1   | 0.96 | 0.11 | -1.47 | 35,35,35,35                | 0     |
| 59  | MG   | BA    | 3229 | 1/1   | 0.96 | 0.13 | -1.75 | 5,5,5,5                    | 0     |
| 59  | MG   | AA    | 1778 | 1/1   | 0.97 | 0.12 | -1.91 | 6,6,6,6                    | 0     |
| 59  | MG   | AA    | 1734 | 1/1   | 0.87 | 0.12 | -2.00 | 41,41,41,41                | 0     |
| 59  | MG   | AA    | 1657 | 1/1   | 0.92 | 0.10 | -2.04 | 32,32,32,32                | 0     |
| 59  | MG   | AA    | 1721 | 1/1   | 0.93 | 0.12 | -2.20 | 17,17,17,17                | 0     |
| 59  | MG   | BA    | 3221 | 1/1   | 0.90 | 0.10 | -2.20 | 43,43,43,43                | 0     |
| 59  | MG   | AA    | 1783 | 1/1   | 0.88 | 0.13 | -2.58 | 43,43,43,43                | 0     |
| 59  | MG   | AA    | 1747 | 1/1   | 0.86 | 0.08 | -2.84 | 23,23,23,23                | 0     |
| 59  | MG   | BA    | 3308 | 1/1   | 0.95 | 0.12 | -2.93 | 58,58,58,58                | 0     |
| 59  | MG   | BA    | 3140 | 1/1   | 0.82 | 0.13 | -3.14 | 45,45,45,45                | 0     |
| 59  | MG   | AA    | 1785 | 1/1   | 0.96 | 0.08 | -3.20 | 47,47,47,47                | 0     |
| 60  | ZN   | B9    | 101  | 1/1   | 1.00 | 0.06 | -3.39 | 49,49,49,49                | 0     |
| 59  | MG   | AY    | 702  | 1/1   | 0.93 | 0.08 | -3.96 | 23,23,23,23                | 0     |
| 59  | MG   | BA    | 3259 | 1/1   | 0.92 | 0.12 | -4.47 | 39,39,39,39                | 0     |
| 59  | MG   | AA    | 1710 | 1/1   | 0.95 | 0.06 | -4.82 | 35,35,35,35                | 0     |
| 59  | MG   | BA    | 3061 | 1/1   | 0.93 | 0.05 | -5.03 | 37,37,37,37                | 0     |
| 59  | MG   | AA    | 1705 | 1/1   | 0.97 | 0.08 | -5.87 | 23,23,23,23                | 0     |
| 59  | MG   | AA    | 1660 | 1/1   | 0.94 | 0.10 | -6.03 | 19,19,19,19                | 0     |
| 59  | MG   | AA    | 1699 | 1/1   | 0.68 | 0.25 | -     | 33,33,33,33                | 0     |
| 59  | MG   | AA    | 1679 | 1/1   | 0.98 | 0.55 | -     | 32,32,32,32                | 0     |
| 59  | MG   | AA    | 1664 | 1/1   | 0.94 | 0.39 | -     | 29,29,29,29                | 0     |
| 59  | MG   | BA    | 3300 | 1/1   | 0.93 | 0.17 | -     | 65,65,65,65                | 0     |
| 59  | MG   | BA    | 3255 | 1/1   | 0.86 | 0.24 | -     | 35,35,35,35                | 0     |
| 59  | MG   | AA    | 1789 | 1/1   | 0.81 | 0.28 | -     | 61,61,61,61                | 0     |
| 59  | MG   | AA    | 1791 | 1/1   | 0.95 | 0.09 | -     | 57,57,57,57                | 0     |
| 59  | MG   | BA    | 3020 | 1/1   | 0.84 | 0.22 | -     | 63,63,63,63                | 0     |
| 59  | MG   | BA    | 3118 | 1/1   | 0.95 | 0.30 | -     | 29,29,29,29                | 0     |
| 59  | MG   | BA    | 3156 | 1/1   | 0.96 | 0.19 | -     | 25,25,25,25                | 0     |
| 59  | MG   | AA    | 1666 | 1/1   | 0.76 | 0.53 | -     | 83,83,83,83                | 0     |
| 59  | MG   | AA    | 1610 | 1/1   | 0.95 | 0.66 | -     | 46,46,46,46                | 0     |
| 59  | MG   | AA    | 1794 | 1/1   | 0.83 | 0.27 | -     | 53,53,53,53                | 0     |
| 59  | MG   | BA    | 3197 | 1/1   | 0.79 | 0.56 | -     | 58,58,58,58                | 0     |
| 59  | MG   | BA    | 3132 | 1/1   | 0.82 | 0.33 | -     | 59,59,59,59                | 0     |
| 59  | MG   | BA    | 3234 | 1/1   | 0.86 | 0.20 | -     | 63,63,63,63                | 0     |
| 59  | MG   | BA    | 3065 | 1/1   | 0.98 | 0.29 | -     | 21,21,21,21                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1748 | 1/1   | 0.85 | 0.36 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3280 | 1/1   | 0.79 | 0.24 | -    | 87,87,87,87                 | 0     |
| 59  | MG   | BA    | 3060 | 1/1   | 0.90 | 0.39 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | AA    | 1753 | 1/1   | 0.66 | 0.53 | -    | 89,89,89,89                 | 0     |
| 59  | MG   | BA    | 3175 | 1/1   | 0.79 | 0.19 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1667 | 1/1   | 0.97 | 0.35 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3106 | 1/1   | 0.84 | 0.22 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | AA    | 1634 | 1/1   | 0.81 | 0.22 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3144 | 1/1   | 0.88 | 0.23 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | AA    | 1768 | 1/1   | 0.87 | 0.46 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3079 | 1/1   | 0.86 | 0.34 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3057 | 1/1   | 0.95 | 0.29 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3166 | 1/1   | 0.80 | 0.28 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | AA    | 1689 | 1/1   | 0.83 | 0.40 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | AA    | 1674 | 1/1   | 0.75 | 0.44 | -    | 74,74,74,74                 | 0     |
| 59  | MG   | BA    | 3018 | 1/1   | 0.89 | 0.56 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3074 | 1/1   | 0.97 | 0.36 | -    | 3,3,3,3                     | 0     |
| 59  | MG   | BA    | 3230 | 1/1   | 0.67 | 0.35 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3224 | 1/1   | 0.96 | 0.46 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3296 | 1/1   | 0.90 | 0.38 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3105 | 1/1   | 0.88 | 0.20 | -    | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3009 | 1/1   | 0.77 | 0.72 | -    | 77,77,77,77                 | 0     |
| 59  | MG   | AA    | 1770 | 1/1   | 0.96 | 0.29 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | AA    | 1694 | 1/1   | 0.93 | 0.13 | -    | 19,19,19,19                 | 0     |
| 59  | MG   | BA    | 3303 | 1/1   | 0.92 | 0.09 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3100 | 1/1   | 0.94 | 0.10 | -    | 24,24,24,24                 | 0     |
| 59  | MG   | AA    | 1707 | 1/1   | 0.81 | 0.22 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3168 | 1/1   | 0.80 | 0.11 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3183 | 1/1   | 0.95 | 0.14 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1683 | 1/1   | 0.92 | 0.23 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | AA    | 1765 | 1/1   | 0.91 | 0.56 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1788 | 1/1   | 0.84 | 0.33 | -    | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3225 | 1/1   | 0.76 | 0.14 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | AA    | 1781 | 1/1   | 0.33 | 0.27 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3242 | 1/1   | 0.73 | 0.44 | -    | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3085 | 1/1   | 0.74 | 0.21 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3249 | 1/1   | 0.96 | 0.31 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | AA    | 1740 | 1/1   | 0.44 | 0.75 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | AA    | 1739 | 1/1   | 0.91 | 0.42 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3016 | 1/1   | 0.72 | 0.62 | -    | 77,77,77,77                 | 0     |
| 59  | MG   | AA    | 1755 | 1/1   | 0.74 | 0.35 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3028 | 1/1   | 0.65 | 0.40 | -    | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1618 | 1/1   | 0.97 | 0.38 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3267 | 1/1   | 0.77 | 0.34 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1603 | 1/1   | 0.94 | 0.41 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1757 | 1/1   | 0.87 | 0.30 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3121 | 1/1   | 0.92 | 0.34 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | AA    | 1659 | 1/1   | 0.97 | 0.39 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1787 | 1/1   | 0.86 | 0.27 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3128 | 1/1   | 0.74 | 0.26 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3134 | 1/1   | 0.87 | 0.31 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3069 | 1/1   | 0.97 | 0.33 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3081 | 1/1   | 0.98 | 0.28 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3095 | 1/1   | 0.81 | 0.38 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3239 | 1/1   | 0.76 | 0.27 | -    | 87,87,87,87                 | 0     |
| 59  | MG   | BA    | 3102 | 1/1   | 0.96 | 0.23 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1626 | 1/1   | 0.92 | 0.42 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3307 | 1/1   | 0.94 | 0.16 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3059 | 1/1   | 0.94 | 0.45 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | AA    | 1779 | 1/1   | 0.63 | 0.53 | -    | 81,81,81,81                 | 0     |
| 59  | MG   | AA    | 1709 | 1/1   | 0.66 | 0.20 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3314 | 1/1   | 0.91 | 0.10 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3198 | 1/1   | 0.88 | 0.17 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3201 | 1/1   | 0.77 | 0.41 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3114 | 1/1   | 0.93 | 0.21 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1769 | 1/1   | 0.91 | 0.36 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | AA    | 1743 | 1/1   | 0.71 | 0.39 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3291 | 1/1   | 0.92 | 0.32 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3170 | 1/1   | 0.93 | 0.52 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | AA    | 1776 | 1/1   | 0.96 | 0.29 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | AA    | 1606 | 1/1   | 0.76 | 0.53 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | AA    | 1730 | 1/1   | 0.96 | 0.13 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1773 | 1/1   | 0.59 | 0.56 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3013 | 1/1   | 0.93 | 0.49 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3220 | 1/1   | 0.93 | 0.18 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | AA    | 1635 | 1/1   | 0.72 | 0.22 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3143 | 1/1   | 0.86 | 0.21 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3241 | 1/1   | 0.90 | 0.19 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3317 | 1/1   | 0.98 | 0.28 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1643 | 1/1   | 0.80 | 0.23 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1764 | 1/1   | 0.79 | 0.27 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3273 | 1/1   | 0.88 | 0.65 | -    | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3131 | 1/1   | 0.97 | 0.43 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3305 | 1/1   | 0.80 | 0.10 | -    | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3163 | 1/1   | 0.84 | 0.30 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | AA    | 1716 | 1/1   | 0.65 | 0.37 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | AA    | 1629 | 1/1   | 0.96 | 0.28 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3179 | 1/1   | 0.37 | 0.43 | -    | 87,87,87,87                 | 0     |
| 59  | MG   | BA    | 3250 | 1/1   | 0.84 | 0.24 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | AA    | 1797 | 1/1   | 0.80 | 0.19 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1767 | 1/1   | 0.88 | 0.29 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3293 | 1/1   | 0.89 | 0.50 | -    | 76,76,76,76                 | 0     |
| 59  | MG   | BA    | 3160 | 1/1   | 0.79 | 0.17 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3063 | 1/1   | 0.97 | 0.15 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | AA    | 1763 | 1/1   | 0.82 | 0.30 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3284 | 1/1   | 0.72 | 0.42 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3202 | 1/1   | 0.90 | 0.40 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | AA    | 1612 | 1/1   | 0.96 | 0.46 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3200 | 1/1   | 0.92 | 0.31 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | AA    | 1670 | 1/1   | 0.92 | 0.21 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3032 | 1/1   | 0.69 | 0.25 | -    | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3205 | 1/1   | 0.95 | 0.12 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3062 | 1/1   | 0.97 | 0.15 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3286 | 1/1   | 0.92 | 0.34 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3212 | 1/1   | 0.88 | 0.28 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1784 | 1/1   | 0.88 | 0.17 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3178 | 1/1   | 0.98 | 0.27 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3086 | 1/1   | 0.95 | 0.26 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1646 | 1/1   | 0.92 | 0.38 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3316 | 1/1   | 0.95 | 0.38 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3047 | 1/1   | 0.96 | 0.37 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1611 | 1/1   | 0.80 | 0.34 | -    | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3015 | 1/1   | 0.89 | 0.53 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1742 | 1/1   | 0.91 | 0.22 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3030 | 1/1   | 0.58 | 1.27 | -    | 86,86,86,86                 | 0     |
| 59  | MG   | AA    | 1752 | 1/1   | 0.90 | 0.22 | -    | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3222 | 1/1   | 0.96 | 0.30 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3019 | 1/1   | 0.55 | 0.72 | -    | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3213 | 1/1   | 0.90 | 0.36 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | B5    | 101  | 1/1   | 0.88 | 0.27 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3027 | 1/1   | 0.88 | 0.30 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | AA    | 1708 | 1/1   | 0.90 | 0.26 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3099 | 1/1   | 0.97 | 0.21 | -    | 19,19,19,19                 | 0     |
| 59  | MG   | AA    | 1631 | 1/1   | 0.94 | 0.20 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3182 | 1/1   | 0.89 | 0.27 | -    | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3042 | 1/1   | 0.81 | 0.37 | -    | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3115 | 1/1   | 0.92 | 0.30 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3049 | 1/1   | 0.92 | 0.46 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3215 | 1/1   | 0.39 | 0.60 | -    | 81,81,81,81                 | 0     |
| 59  | MG   | AA    | 1627 | 1/1   | 0.86 | 0.23 | -    | 74,74,74,74                 | 0     |
| 59  | MG   | BA    | 3185 | 1/1   | 0.91 | 0.43 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3309 | 1/1   | 0.96 | 0.17 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1642 | 1/1   | 0.86 | 0.26 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | AA    | 1662 | 1/1   | 0.90 | 0.33 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3055 | 1/1   | 0.83 | 0.16 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3287 | 1/1   | 0.92 | 0.17 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | AA    | 1644 | 1/1   | 0.69 | 0.20 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | AA    | 1614 | 1/1   | 0.96 | 0.40 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | AA    | 1669 | 1/1   | 0.86 | 0.20 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3223 | 1/1   | 0.95 | 0.34 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1798 | 1/1   | 0.87 | 0.07 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3247 | 1/1   | 0.37 | 0.37 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1720 | 1/1   | 0.95 | 0.47 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | AA    | 1602 | 1/1   | 0.88 | 0.48 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1782 | 1/1   | 0.96 | 0.09 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | BC    | 301  | 1/1   | 0.66 | 0.21 | -    | 115,115,115,115             | 0     |
| 59  | MG   | AA    | 1605 | 1/1   | 0.94 | 0.42 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | AA    | 1619 | 1/1   | 0.96 | 0.36 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3068 | 1/1   | 0.91 | 0.19 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | AA    | 1632 | 1/1   | 0.64 | 0.25 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3194 | 1/1   | 0.38 | 0.35 | -    | 74,74,74,74                 | 0     |
| 59  | MG   | BA    | 3133 | 1/1   | 0.87 | 0.31 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3211 | 1/1   | 0.91 | 0.65 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3107 | 1/1   | 0.83 | 0.30 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3096 | 1/1   | 0.97 | 0.20 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3136 | 1/1   | 0.64 | 0.30 | -    | 90,90,90,90                 | 0     |
| 59  | MG   | BA    | 3036 | 1/1   | 0.83 | 0.28 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3276 | 1/1   | 0.77 | 0.51 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1654 | 1/1   | 0.92 | 0.26 | -    | 24,24,24,24                 | 0     |
| 59  | MG   | BA    | 3292 | 1/1   | 0.80 | 0.36 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3072 | 1/1   | 0.84 | 0.63 | -    | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3187 | 1/1   | 0.81 | 0.89 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3256 | 1/1   | 0.95 | 0.44 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1723 | 1/1   | 0.96 | 0.14 | -    | 10,10,10,10                 | 0     |
| 59  | MG   | BA    | 3245 | 1/1   | 0.95 | 0.23 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | AA    | 1655 | 1/1   | 0.94 | 0.40 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1651 | 1/1   | 0.88 | 0.20 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3148 | 1/1   | 0.81 | 0.29 | -    | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1607 | 1/1   | 0.74 | 0.34 | -    | 97,97,97,97                 | 0     |
| 59  | MG   | AA    | 1681 | 1/1   | 0.96 | 0.45 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3191 | 1/1   | 0.89 | 0.38 | -    | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3119 | 1/1   | 0.98 | 0.26 | -    | 24,24,24,24                 | 0     |
| 59  | MG   | BA    | 3002 | 1/1   | 0.98 | 0.13 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | AA    | 1717 | 1/1   | 0.94 | 0.43 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3083 | 1/1   | 0.97 | 0.42 | -    | 23,23,23,23                 | 0     |
| 59  | MG   | AA    | 1637 | 1/1   | 0.68 | 0.58 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1790 | 1/1   | 0.77 | 0.25 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3124 | 1/1   | 0.99 | 0.27 | -    | 15,15,15,15                 | 0     |
| 59  | MG   | BA    | 3251 | 1/1   | 0.83 | 0.28 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3192 | 1/1   | 0.92 | 0.36 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3123 | 1/1   | 0.98 | 0.49 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3301 | 1/1   | 0.91 | 0.41 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | AA    | 1696 | 1/1   | 0.88 | 0.35 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3195 | 1/1   | 0.94 | 0.25 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3005 | 1/1   | 0.97 | 0.48 | -    | 16,16,16,16                 | 0     |
| 59  | MG   | AA    | 1795 | 1/1   | 0.96 | 0.15 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3265 | 1/1   | 0.71 | 0.55 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1672 | 1/1   | 0.93 | 0.18 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3126 | 1/1   | 0.84 | 0.42 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3158 | 1/1   | 0.95 | 0.30 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1758 | 1/1   | 0.77 | 0.39 | -    | 75,75,75,75                 | 0     |
| 59  | MG   | AA    | 1745 | 1/1   | 0.80 | 0.44 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | AA    | 1621 | 1/1   | 0.80 | 0.40 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3270 | 1/1   | 0.83 | 0.34 | -    | 70,70,70,70                 | 0     |
| 59  | MG   | AA    | 1766 | 1/1   | 0.76 | 0.29 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1744 | 1/1   | 0.80 | 0.21 | -    | 90,90,90,90                 | 0     |
| 59  | MG   | BA    | 3089 | 1/1   | 0.92 | 0.24 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3029 | 1/1   | 0.87 | 0.33 | -    | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3173 | 1/1   | 0.95 | 0.27 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | AA    | 1695 | 1/1   | 0.78 | 0.34 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1656 | 1/1   | 0.87 | 0.15 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3025 | 1/1   | 0.74 | 0.32 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3067 | 1/1   | 0.79 | 0.28 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | AA    | 1775 | 1/1   | 0.91 | 0.13 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3235 | 1/1   | 0.96 | 0.20 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1714 | 1/1   | 0.69 | 0.53 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3254 | 1/1   | 0.91 | 0.27 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3281 | 1/1   | 0.41 | 0.46 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | AA    | 1727 | 1/1   | 0.90 | 0.14 | -    | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3146 | 1/1   | 0.89 | 0.23 | -    | 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   | BA    | 3092 | 1/1   | 0.96 | 0.59 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3041 | 1/1   | 0.82 | 0.21 | -    | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3268 | 1/1   | 0.58 | 0.35 | -    | 85,85,85,85                 | 0     |
| 59  | MG   | AA    | 1617 | 1/1   | 0.96 | 0.49 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3193 | 1/1   | 0.81 | 0.53 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3022 | 1/1   | 0.91 | 0.55 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3152 | 1/1   | 0.94 | 0.41 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3285 | 1/1   | 0.91 | 0.28 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | AA    | 1728 | 1/1   | 0.77 | 0.32 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3026 | 1/1   | 0.77 | 0.36 | -    | 67,67,67,67                 | 0     |
| 59  | MG   | AA    | 1620 | 1/1   | 0.85 | 0.44 | -    | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3101 | 1/1   | 0.97 | 0.35 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3080 | 1/1   | 0.98 | 0.41 | -    | 38,38,38,38                 | 0     |
| 59  | MG   | AA    | 1698 | 1/1   | 0.85 | 0.31 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1786 | 1/1   | 0.88 | 0.15 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1624 | 1/1   | 0.85 | 0.84 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3130 | 1/1   | 0.92 | 0.55 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3038 | 1/1   | 0.93 | 0.31 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3311 | 1/1   | 0.96 | 0.35 | -    | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3240 | 1/1   | 0.69 | 0.33 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3216 | 1/1   | 0.91 | 0.20 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3064 | 1/1   | 0.77 | 0.12 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3012 | 1/1   | 0.64 | 0.44 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | AA    | 1754 | 1/1   | 0.57 | 0.40 | -    | 75,75,75,75                 | 0     |
| 59  | MG   | AA    | 1796 | 1/1   | 0.79 | 0.28 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3204 | 1/1   | 0.42 | 0.40 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3031 | 1/1   | 0.92 | 0.35 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1691 | 1/1   | 0.84 | 0.11 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3070 | 1/1   | 0.98 | 0.45 | -    | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3093 | 1/1   | 0.91 | 0.42 | -    | 69,69,69,69                 | 0     |
| 59  | MG   | AA    | 1650 | 1/1   | 0.76 | 0.26 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | AA    | 1772 | 1/1   | 0.88 | 0.58 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | BA    | 3299 | 1/1   | 0.86 | 0.41 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3165 | 1/1   | 0.99 | 0.45 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1647 | 1/1   | 0.75 | 0.46 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | BA    | 3306 | 1/1   | 0.94 | 0.23 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | AA    | 1706 | 1/1   | 0.95 | 0.16 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3040 | 1/1   | 0.79 | 0.42 | -    | 71,71,71,71                 | 0     |
| 59  | MG   | AA    | 1759 | 1/1   | 0.97 | 0.33 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3138 | 1/1   | 0.88 | 0.47 | -    | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3177 | 1/1   | 0.95 | 0.40 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3090 | 1/1   | 0.89 | 0.32 | -    | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3304 | 1/1   | 0.67 | 0.39 | -    | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3003 | 1/1   | 0.96 | 0.35 | -    | 20,20,20,20                 | 0     |
| 59  | MG   | AA    | 1712 | 1/1   | 0.43 | 0.23 | -    | 66,66,66,66                 | 0     |
| 59  | MG   | AA    | 1750 | 1/1   | 0.93 | 0.30 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3190 | 1/1   | 0.67 | 0.38 | -    | 81,81,81,81                 | 0     |
| 59  | MG   | AA    | 1735 | 1/1   | 0.89 | 0.41 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3218 | 1/1   | 0.77 | 0.23 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3264 | 1/1   | 0.76 | 0.56 | -    | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3278 | 1/1   | 0.96 | 0.24 | -    | 91,91,91,91                 | 0     |
| 59  | MG   | AA    | 1702 | 1/1   | 0.97 | 0.53 | -    | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3263 | 1/1   | 0.63 | 0.33 | -    | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1688 | 1/1   | 0.94 | 0.25 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3011 | 1/1   | 0.94 | 0.27 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3237 | 1/1   | 0.84 | 0.20 | -    | 94,94,94,94                 | 0     |
| 59  | MG   | AA    | 1622 | 1/1   | 0.91 | 0.47 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1731 | 1/1   | 0.87 | 0.09 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1703 | 1/1   | 0.72 | 0.42 | -    | 81,81,81,81                 | 0     |
| 59  | MG   | BA    | 3260 | 1/1   | 0.80 | 0.46 | -    | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3017 | 1/1   | 0.96 | 0.33 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3283 | 1/1   | 0.81 | 0.21 | -    | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3147 | 1/1   | 0.72 | 0.55 | -    | 119,119,119,119             | 0     |
| 59  | MG   | BA    | 3238 | 1/1   | 0.86 | 0.28 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3272 | 1/1   | 0.94 | 0.43 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1676 | 1/1   | 0.82 | 0.24 | -    | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3066 | 1/1   | 0.97 | 0.16 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1675 | 1/1   | 0.96 | 0.27 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3274 | 1/1   | 0.88 | 0.18 | -    | 79,79,79,79                 | 0     |
| 59  | MG   | BA    | 3294 | 1/1   | 0.94 | 0.20 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1648 | 1/1   | 0.91 | 0.35 | -    | 29,29,29,29                 | 0     |
| 59  | MG   | BU    | 201  | 1/1   | 0.92 | 0.14 | -    | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3164 | 1/1   | 0.88 | 0.24 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1601 | 1/1   | 0.81 | 0.23 | -    | 97,97,97,97                 | 0     |
| 59  | MG   | BA    | 3046 | 1/1   | 0.89 | 0.28 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1718 | 1/1   | 0.95 | 0.50 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1663 | 1/1   | 0.85 | 0.47 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3290 | 1/1   | 0.94 | 0.42 | -    | 43,43,43,43                 | 0     |
| 59  | MG   | AA    | 1640 | 1/1   | 0.79 | 0.26 | -    | 74,74,74,74                 | 0     |
| 59  | MG   | BA    | 3227 | 1/1   | 0.92 | 0.28 | -    | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1641 | 1/1   | 0.97 | 0.17 | -    | 17,17,17,17                 | 0     |
| 59  | MG   | AA    | 1713 | 1/1   | 0.92 | 0.16 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3045 | 1/1   | 0.81 | 0.69 | -    | 54,54,54,54                 | 0     |
| 59  | MG   | AA    | 1658 | 1/1   | 0.89 | 0.19 | -    | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3162 | 1/1   | 0.89 | 0.26 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3203 | 1/1   | 0.94 | 0.27 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1737 | 1/1   | 0.86 | 0.18 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3117 | 1/1   | 0.90 | 0.19 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3159 | 1/1   | 0.97 | 0.20 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3035 | 1/1   | 0.97 | 0.51 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | AA    | 1628 | 1/1   | 0.53 | 0.42 | -    | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3233 | 1/1   | 0.86 | 0.20 | -    | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3252 | 1/1   | 0.39 | 0.60 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3135 | 1/1   | 0.95 | 0.25 | -    | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3023 | 1/1   | 0.90 | 0.12 | -    | 87,87,87,87                 | 0     |
| 59  | MG   | BA    | 3302 | 1/1   | 0.89 | 0.39 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1661 | 1/1   | 0.86 | 0.29 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | AA    | 1680 | 1/1   | 0.96 | 0.19 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3137 | 1/1   | 0.86 | 0.16 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3320 | 1/1   | 0.98 | 0.13 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3155 | 1/1   | 0.72 | 0.29 | -    | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3188 | 1/1   | 0.93 | 0.41 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1613 | 1/1   | 0.91 | 0.18 | -    | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3253 | 1/1   | 0.84 | 0.40 | -    | 98,98,98,98                 | 0     |
| 59  | MG   | BA    | 3167 | 1/1   | 0.86 | 0.17 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3037 | 1/1   | 0.90 | 0.40 | -    | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1630 | 1/1   | 0.88 | 0.53 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3262 | 1/1   | 0.90 | 0.15 | -    | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3054 | 1/1   | 0.87 | 0.28 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3010 | 1/1   | 0.98 | 0.41 | -    | 33,33,33,33                 | 0     |
| 59  | MG   | AA    | 1792 | 1/1   | 0.81 | 0.12 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3103 | 1/1   | 0.97 | 0.20 | -    | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1685 | 1/1   | 0.92 | 0.42 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3246 | 1/1   | 0.94 | 0.31 | -    | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1608 | 1/1   | 0.87 | 0.37 | -    | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3226 | 1/1   | 0.82 | 0.34 | -    | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3014 | 1/1   | 0.96 | 0.34 | -    | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3008 | 1/1   | 0.96 | 0.46 | -    | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3034 | 1/1   | 0.96 | 0.25 | -    | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3231 | 1/1   | 0.97 | 0.34 | -    | 13,13,13,13                 | 0     |
| 59  | MG   | AA    | 1697 | 1/1   | 0.80 | 0.12 | -    | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3112 | 1/1   | 0.85 | 0.71 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3275 | 1/1   | 0.65 | 0.38 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1746 | 1/1   | 0.90 | 0.39 | -    | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3261 | 1/1   | 0.83 | 0.14 | -    | 67,67,67,67                 | 0     |
| 59  | MG   | AA    | 1771 | 1/1   | 0.75 | 0.23 | -    | 40,40,40,40                 | 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   | 0.98 | 0.21 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | AA    | 1609 | 1/1   | 0.95 | 0.42 | -    | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3297 | 1/1   | 0.92 | 0.18 | -    | 39,39,39,39                 | 0     |
| 59  | MG   | AA    | 1793 | 1/1   | 0.86 | 0.23 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3076 | 1/1   | 0.98 | 0.29 | -    | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3058 | 1/1   | 0.97 | 0.31 | -    | 31,31,31,31                 | 0     |
| 59  | MG   | AA    | 1774 | 1/1   | 0.91 | 0.62 | -    | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3021 | 1/1   | 0.96 | 0.32 | -    | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3318 | 1/1   | 0.99 | 0.08 | -    | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1652 | 1/1   | 0.94 | 0.44 | -    | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3122 | 1/1   | 0.89 | 0.17 | -    | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3186 | 1/1   | 0.86 | 0.15 | -    | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1633 | 1/1   | 0.95 | 0.54 | -    | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3161 | 1/1   | 0.95 | 0.42 | -    | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3073 | 1/1   | 0.88 | 0.33 | -    | 83,83,83,83                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.